PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Spray Wall Interactions and Soot Formation

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Annual Merit Review, 2 June 2020, 11:30 am EDT,
Project ACE144

Overview: spray wall interactions and soot formation

- **Timeline**
  - All projects started mid-2019 and are expected to continue to 2023

	Task	Description
experimental	D.01.05 Pickett	SNL, Free spray and wall film optical experiments Pickett, Skeen, Manin, Hwang, Cenker, Maes
experimental	D.01.04 Manin	SNL, Soot and film combustion Manin, Skeen, Pickett, Cenker, Maes, Sim
experimental	E.01.02 Sjöberg	SNL, DISI metal and optical engine experiments Sjöberg, Kim, Vuilleumier, Reuss
experimental	D.01.01 Powell	ANL, Free spray and wall film x-ray experiments Powell, Sforzo, Tekawade
experimental	D.01.02 Wissink	ORNL, Spray impingement and wall film neutron imaging experiments; Wissink
modeling	D.01.03 Nguyen	SNL, Evaporative free spray and soot film combustion modeling; Nguyen, Tagliente, Pickett, Chen
modeling	D.02.01 Torelli	ANL, GDI spray-wall interaction modeling Torelli, Som
modeling	D.02.04 Waters	LANL, Multi-phase Lagrangian-Eulerian methods and models for sprays and films: Waters, Carrington, Mahamud, Jariwala
	D.01.06 Pickett	SNL, Spray team coordination, data sharing, ECN lead Pickett, Maes, Hwang, Prisbrey, Nguyen, Tagliante

Funded tasks are divided between different AMR presentations, including ACE 143 Powell. See total budgets in Appendix

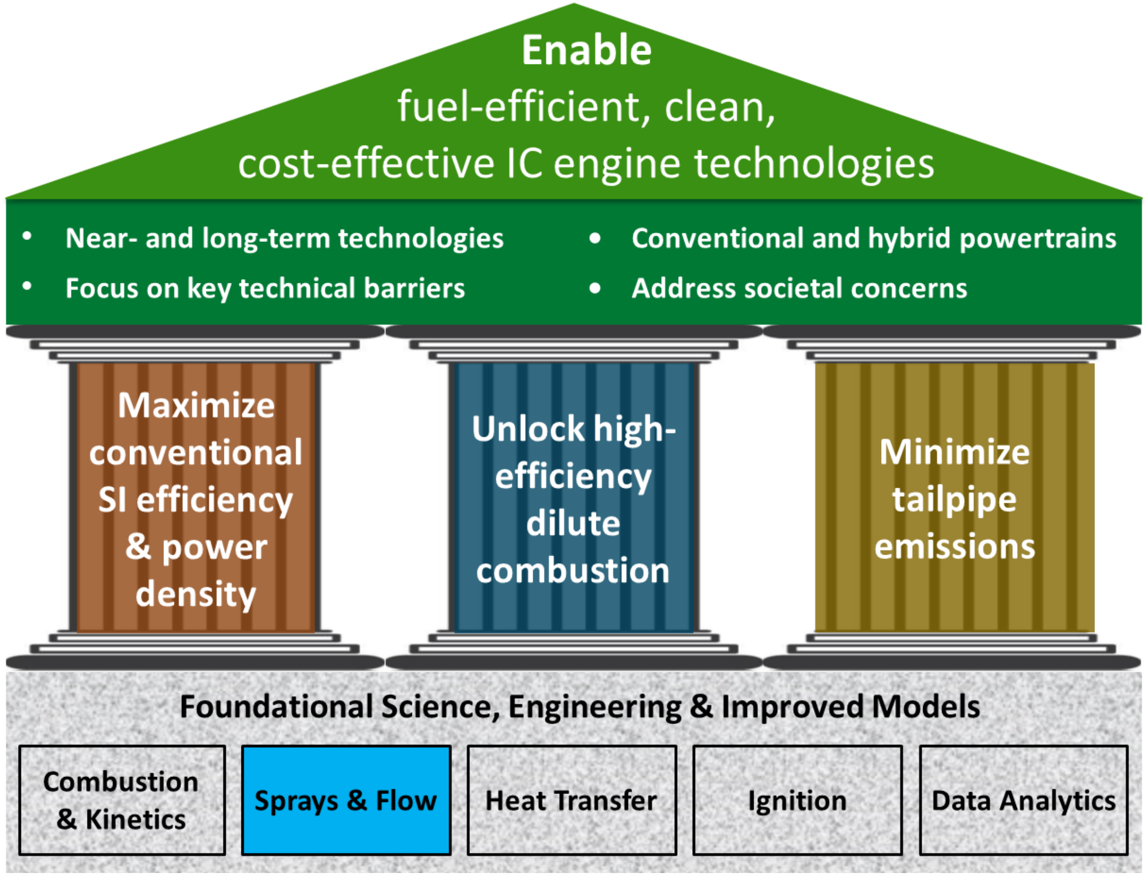
- **Addresses all major PACE outcomes/goals**
  - Minimizing emissions at all operating conditions, including cold-start with potential film combustion
  - Predicting free-spray and wall-impinging sprays, ultimately producing combustible mixtures at the spark plug for efficient (including dilute) combustion
  - Avoiding liner and piston liquid impingement, with implications on knock and premixed ignition
  - CFD spray and film combustion model improvement for engine design/optimization

- **Partners**
  - 15 Industry partners in the AEC MOU
  - PACE sprays team coordinates tasks and sets direction
  - PACE linkages to cold-start, combustion, surrogates,..
  - Engine Combustion Network, Spray G (20+ partners)
  - Convergent Science Inc. software
  - FEARCE software
  - + Many more discussed in slides

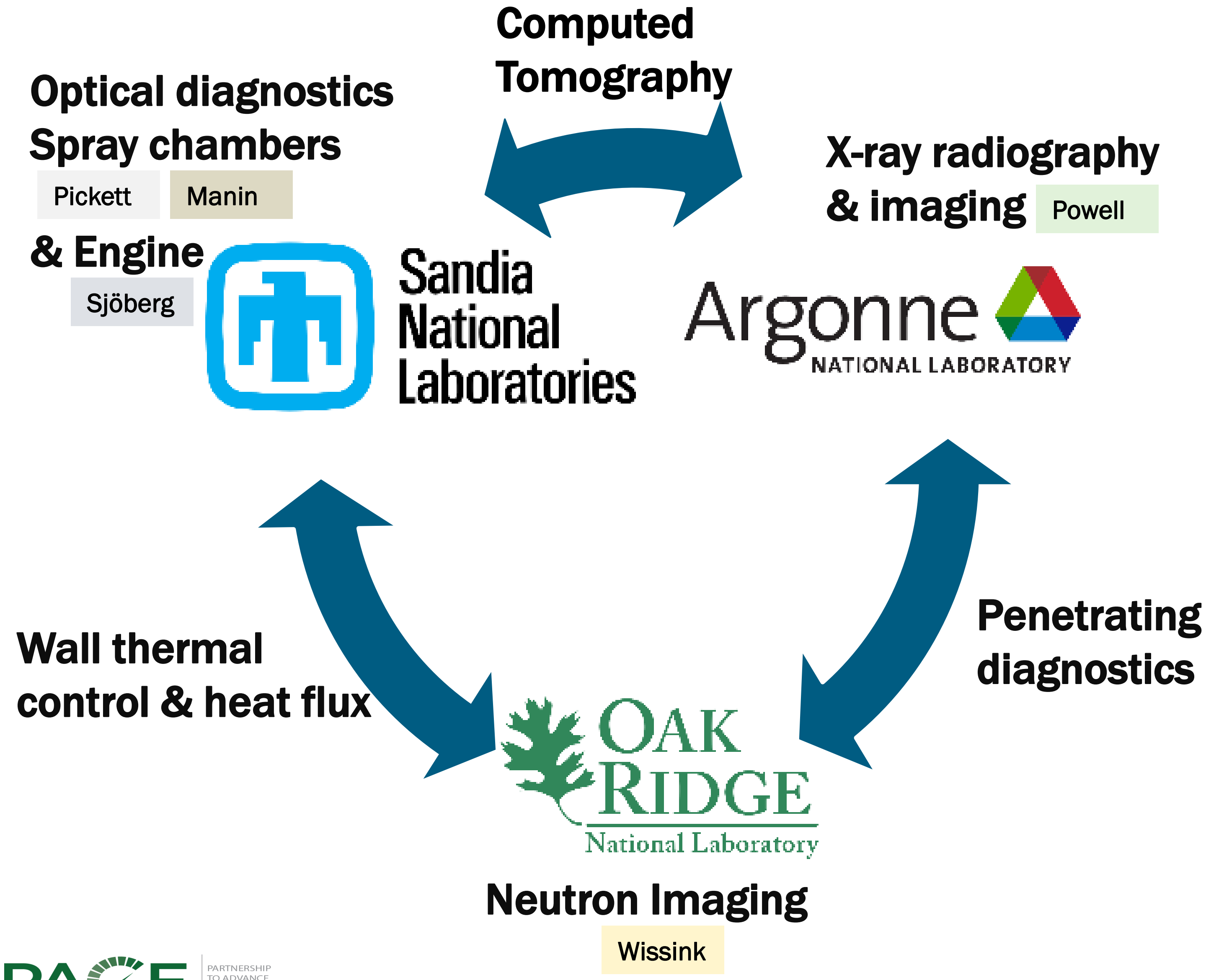
Relevance: Major Outcomes of PACE and the Role of the Sprays Team

Improved understanding and modeling of sprays, films, and mixture formation addresses

- **Ability to Predict and Mitigate Knock and Pre-ignition at High Load**
  - Simulation and experiments characterizing free sprays, wall impingement, and mixture formation
- **Overcome Barriers to Lean/Dilute Combustion**
  - Measurements and modeling of mixture formation under lean/dilute conditions
  - Measure and model spray variability
- **Minimize tailpipe emissions**
  - Experiments and modeling including multiple injections at cold-start conditions
  - Modeling of spray-wall interactions, films, vaporization, heat transfer, wall-film soot
  - How to create a combustible mixture at the spark plug on Cycle 1?

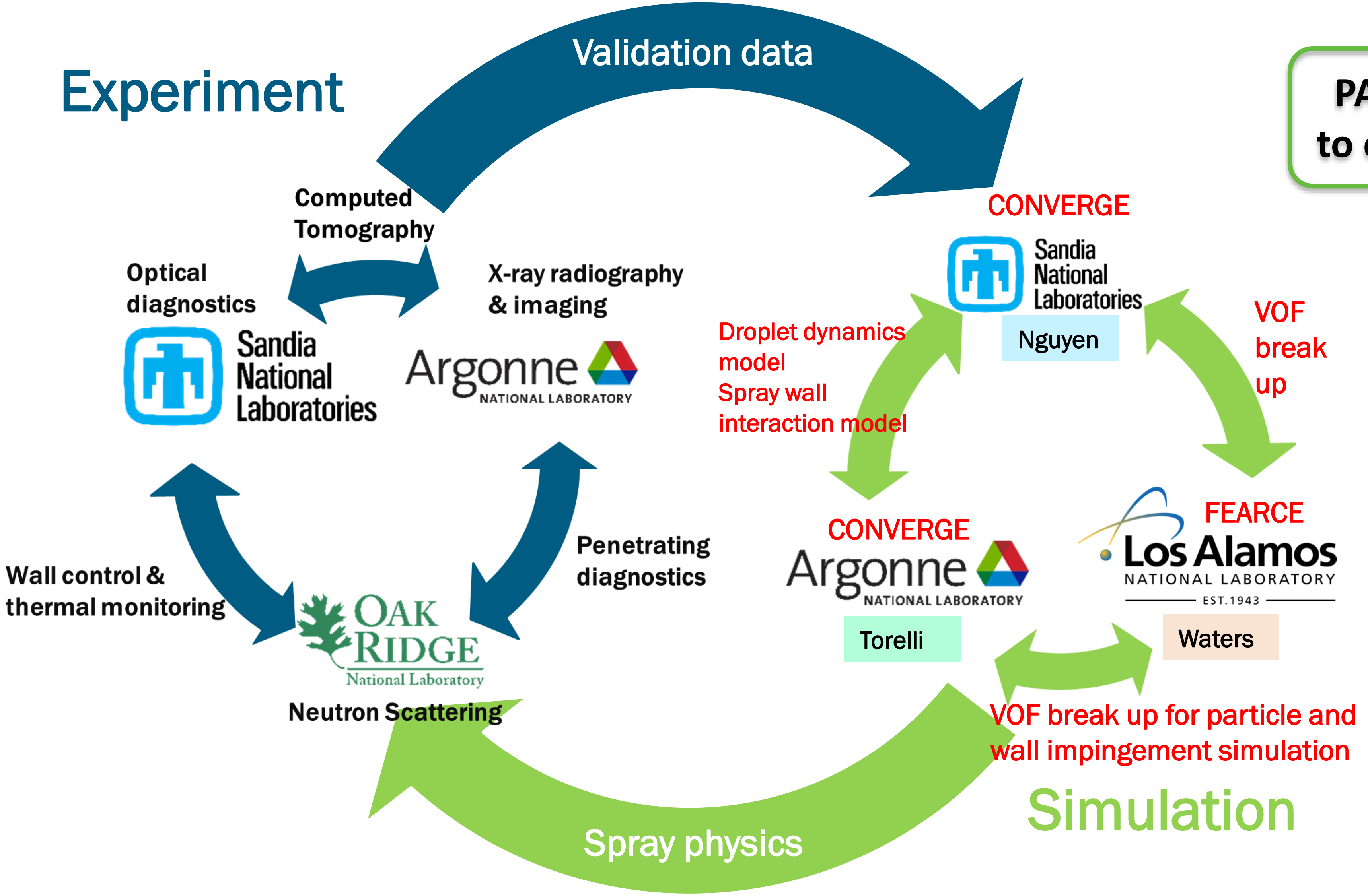


Overall Experimental Approach



- **Focusing on gasoline free spray and impingement phenomena**
- **Free sprays must remain a focus to**
  - Avoid wall impingement if possible
  - Have proper understanding of spray at time of wall impact
- **Coordinated experimental design**
- **Complementary diagnostics**
- **Deliver detailed validation data for CFD simulations**
  - **Impingement process and outcomes must be predicted to design an engine to avoid it!**

Overall modeling approach, tied to experiments



PACE Sprays Team meets monthly to coordinate over 60 current tasks:

- Focusing on gasoline free spray and impingement phenomena
- Simulations at target conditions with different modeling assumptions, compared to unique validation data
- Identify key weaknesses in spray and film models and take action to fix these weaknesses

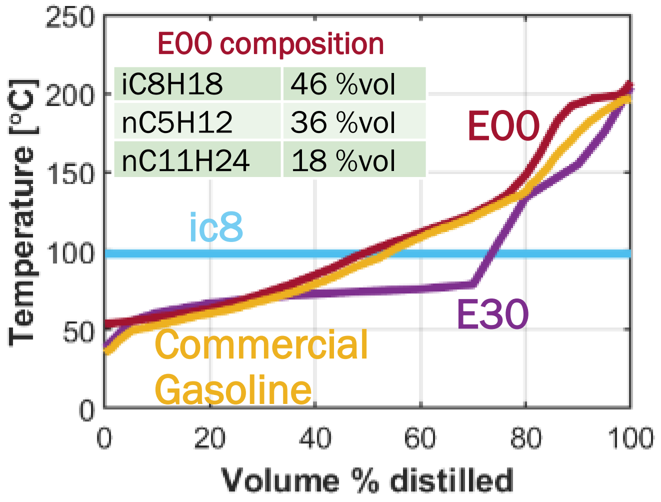
Free-spray target conditions: chosen for joint PACE research to "lay" the foundation for wall-film research at similar conditions

Operating conditions of interest for GDI applications

	T_{amb} [K]	P_{amb} [kPa-a]	ρ_{amb} [kg/m^3]	T_f [K]	p_{inj} [MPa]	$T_{inj,hyd}$ [ms]	m_{inj} [mg]
G1	573	600	3.5	363	20	0.780	10
G2	333	50	0.5	363	20	0.780	10
G3	333	100	1.01	363	20	0.780	10
G2-cold	293	50	0.57	293	20	0.780	10
G3-cold	293	100	1.15	293	20	0.780	10
G3-double	333	100	1.01	363	20	0.462 0.900 dwell 0.327	6 + 4
G1-E00	573	600	3.5	363	20	0.780	10
G2-E00	333	50	0.5	363	20	0.780	10
G3-E00	333	100	1.01	363	20	0.780	10
G2-cold-E00	293	50	0.57	293	20	0.780	10
G3-cold-E00	293	100	1.15	293	20	0.780	10

Overview

- **Injector: ECN Spray G, 8-hole unit provided by Delphi**
- **Fuel: iso-octane/E00 three-component fuel**
- **Ambient: 100% N2**
- **Multi-component fuel is needed to match gasoline**
- **Using fuel proposed by Cordier et al. IJER 2019 with preferential evaporation measurements available**



<u>Importance of operating conditions </u>(many are ECN conditions)

G1: injection late during compression

- **knock control, lean dilute combustion, cold start**

G2: intake injection commonly encountered

- **flash-boiling; modeling weaknesses demonstrated**

G3: intake injection at 1 bar

- **standard patternator and other SAE J2715 data available**

double injection and cold fuel are applicable to cold start

Milestones (1)

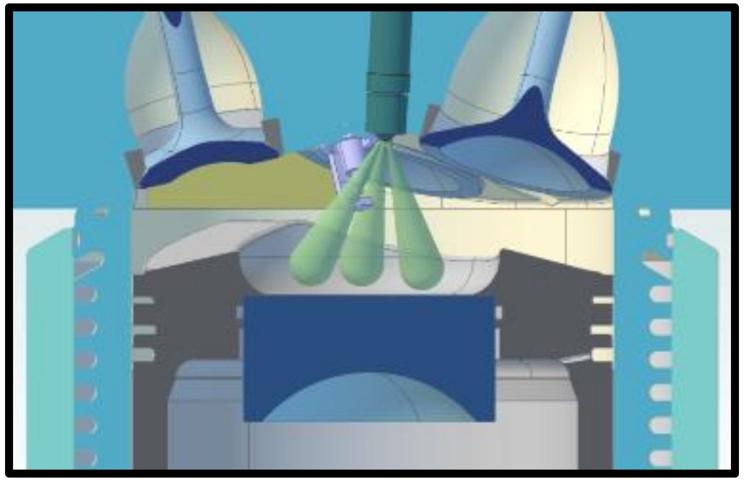
Project	Month/ Year	Description	Status
D.01.05 Pickett	Nov 2019	Provide free-spray dataset on time-resolved 3D liquid volume fraction with measurements well past wall impingement positions. Dataset is for ECN Spray G at 12 conditions, including temperature, pressure, fuel variation.	Posted to ECN
D.01.04 Manin	Sept 2019	Quantify soot formation from fuel films deposited on wall in constant-volume combustion vessel under stoichiometric operation.	Complete
E.01.02 Sjöberg	Nov 2019	Perform scoping study in optical DISI engine to bracket/identify multiple-injection conditions likely used for cold-start operation	Complete
D.01.01 Powell	Mar 2020	Submit free-spray and wall-jet measurements results to the 7th ECN Workshop for comparison with simulation predictions	Complete
D.01.02 Wissink	Sept 2019	Modify wall design and pressure chamber for neutron beam access through specific wall and impingement sections.	Complete
D.01.03 Nguyen	Dec 2019	Implement corrected droplet distortion model in CONVERGE and validate for both diesel and gasoline injection.	Complete
D.02.01 Torelli	Dec 2019	Validation of recently developed spray-wall interaction model against x-ray measurements under GDI G2, G3 conditions	75% (porting to CONVERGE 3.0)
D.02.04 Waters	Sept 2019	Development of A Multi-phase Lagrangian-Eulerian method for sprays and films. Model development and validation of free-sprays on different cases.	Phase 1 Complete
D.01.06 Pickett	Feb 2020	Lead ECN and synthesis activities for experiments and simulations, resulting in "workshop format" sharing\evaluation of final results/analysis/conclusions at Feb AEC meeting	Complete

Milestones (2) through end of FY20

Project	Month/ Year	Description	Status
D.01.05 Pickett	Aug 2020	Complete construction of temperature-controlled wall with optical access and heat flux probe mounted inside pressure chamber	Design under revision
D.01.04 Manin	Sept 2020	Measure soot formation due to spray collapse with wall impingement and with laser ignition	In progress
E.01.02 Sjöberg	June 2020	In DISI engine, perform optical diagnostics to directly assess effects of engine flows on spray development / collapse	on track
D.01.01 Powell	Sept 2020	Dataset of measurement results including free-spray and wall-film measurements archived	on track
D.01.02 Wissink			
D.01.03 Nguyen	July 2020	Wall impingement simulation for Spray G and single-hole injector, incorporating improved free-spray modeling	Setting up
D.02.01 Torelli	March 2020	Validation of recently developed spray-wall interaction model against x-ray measurements under GDI cold-start conditions	75% (porting to CONVERGE 3.0)
D.02.04 Waters	Sept 2020	1. Better evaporation model combined with VOF for phase changes (liquid to gas accounting for mass and heat transfer). 2. Free spray with cross flow at more realistic conditions and introducing true multi-phase Eulerian-Lagrangian modeling fluid in and from injector for more predictive phase-space conditions of Lagrangian spray model.	testing phase
D.01.06 Pickett	July 2020	Manage release of multiple experimental and simulation datasets to ECN archive leading up to ECN7 and afterwards	In progress

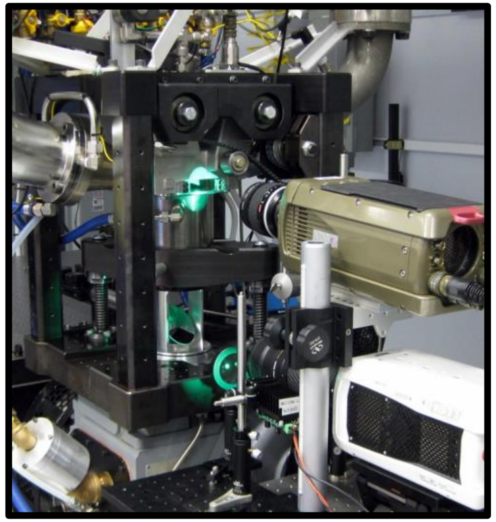
Approach: Sandia Direct-Injection Spark-Ignition Engine

- Drop-down single-cylinder engine.
  Bore: 86 mm, Stroke: 95 mm, CR:12, 0.55L.
- Piston bowl and closely located spark and injector. Early injections for "well-mixed" oper.

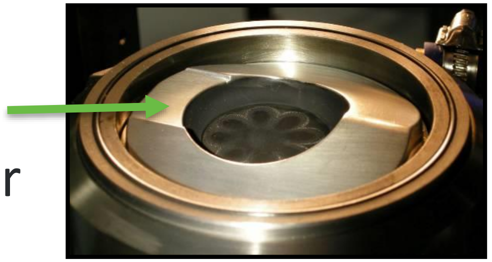


- Identical geometry for all-metal testing and optical diagnostics.
  - Mie or DBI - Liquid Spray, Flame imaging - Deflagration and Soot, DBI - Soot Mass, RIM - Wall Wetting, IR - Fuel Vapor, PIV - Flows.

- First, conduct performance testing with all-metal engine over wide ranges of conditions; skip-fired cold to steady-state warm.
- ACEC Cold-Start protocol is a part of the test matrix.
- Measure PM and PN.
- Second, apply optical diagnostics to:
- Visualize spray dynamics and wall impingement.



- Determine dominating soot-production pathways; *e.g.* bulk soot, piston-top pool fires, injector tip flames.
- Assess the effect of fouling of injector tip and in-cylinder surfaces on PM magnitude.



Stoichiometric cold-start operation with regular gasoline clearly shows the need to avoid wall-wetting and film combustion

- ACEC Cold-Start protocol with E10 RD5-87 fuel used as a starting point for parametric studies.
- 1300 rpm, $\lambda = 1$, 20 mg fuel + 282 mg air / cycle $\Rightarrow$ exhaust enthalpy 4.3 kW/liter for cat. heating.
- Expanded test matrix with other engine thermal states and various injection schedules.
- Steady firing vs. skip-fire $\Rightarrow$ changes surface temperature. Double injection shows very high sensitivity to the thermal state $\Rightarrow$ x80 PM level.
- Engine results serve as guidance for spray-vessel experiments. $P_{intake} \approx 50$ kPa.
- In-cylinder imaging reveals several pathways for soot PM:

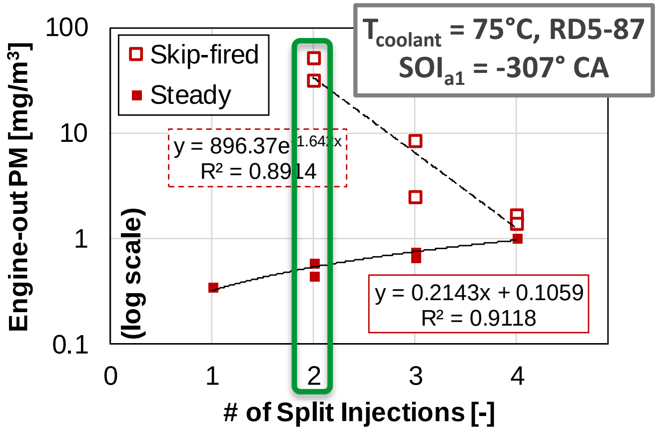
A. Spray-wall interactions cause sooting pool-fires.

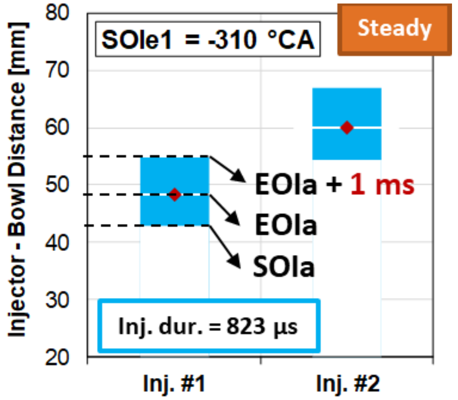
B. Bulk-gas soot, especially for cold conditions with poor atomization.

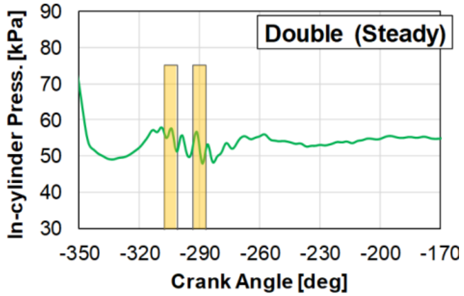
C. Injector-tip wetting and diffusion flames.

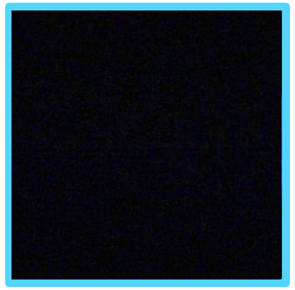
- Effect of tip fouling being assessed.

- **Need to avoid all soot pathways for clean combustion.**



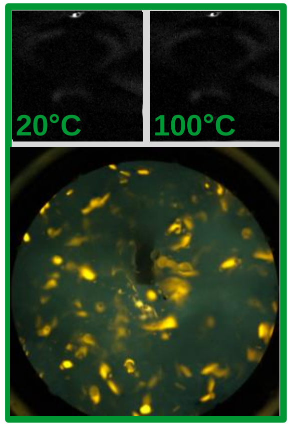






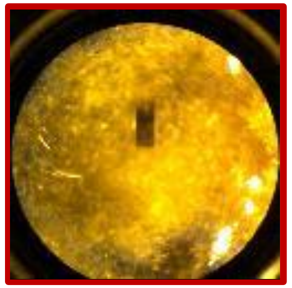
Design Target = Cleanest

Injector-tip diffusion flames



Bulk Soot

Piston-top pool fires



Sootiest

PACE target conditions for future spray-wall research in chambers

- **Optical engine experiments guide initial selection of specific wall target operating conditions**

Sjöberg

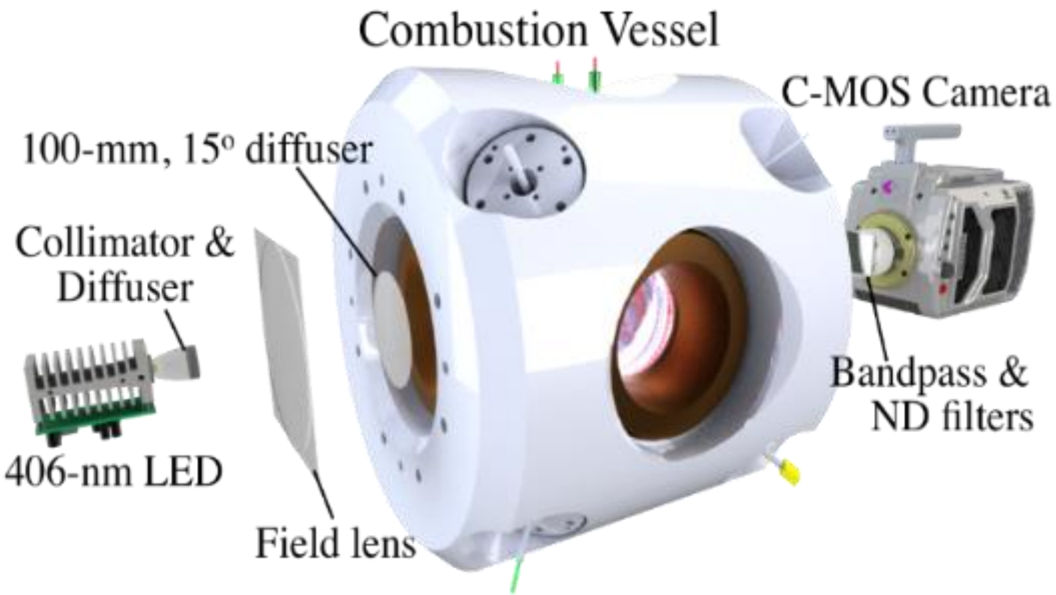
  - Cold-start catalyst heating focus, with skip-firing producing colder walls
  - Enrichment on cycle 1
  - Double injection (or more)
  - Sub-atmospheric pressure (50 kPa absolute)
  - Multi-component surrogate representative of gasoline required

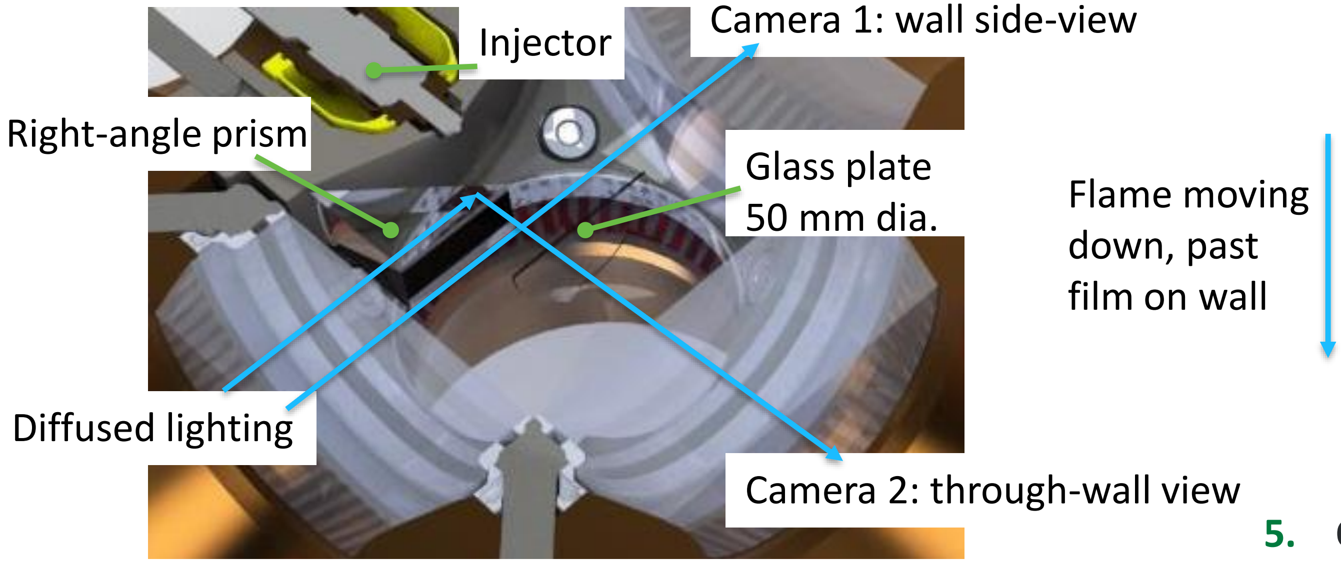
Condition Name	Ambient T (K)	Ambient P (kPa)	Fuel T (K)	Fuel P (MPa)	Fuel Mass (mg/inj)	Fuel	Wall Position	Wall T (K)
W1-C-Cycle10	293	50	293	20	10+10 = 20	PACE surrogate	40 mm	298 (TBD)
W1-C-Cycle1	293	50	293	20	15+15 = 30	PACE surrogate	40 mm	298 (TBD)
W2-2080-Cycle1	305 (TBD)	50	305 (TBD)	20	10+10 = 20	PACE surrogate	40 mm	323 (TBD)
W2-2080-Cycle1-W60	305 (TBD)	50	305 (TBD)	20	10+10 = 20	PACE surrogate	60 mm	323 (TBD)

…other conditions to be defined

- **Spray wall experiments and simulations to date represent proof of concept, rather than the conditions above. Experiments and simulations are not yet unified across the spray team.**

Sandia spray-wall impingement, combustion, and soot quantification (from wall film)

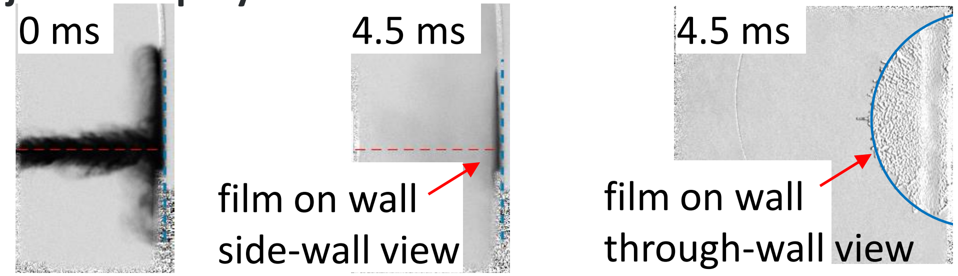




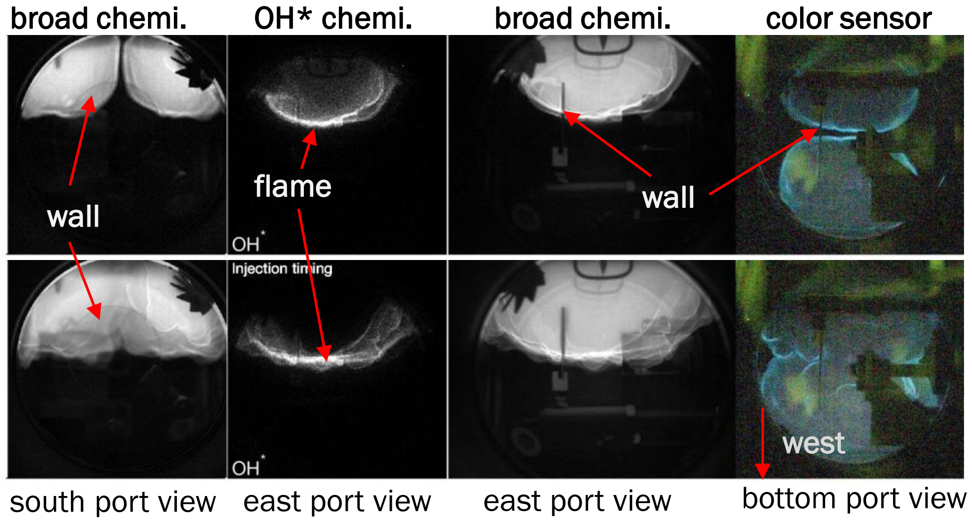
Simultaneous extinction imaging for soot (and liquid) in two views

Steps of film combustion experiment:

1. **Prepare chamber with stoichiometric reactants in chamber**
2. **Spark ignite at two locations at top of chamber**
3. **Inject fuel spray to form film on flat wall at x = 50 mm**



4. **Observe flame passing over film, in analog to engine combustion with fuel films on surfaces**



5. **Quantify soot formation in simultaneous lines of sight “along” wall and “through” wall**

Processes of film formation and evaporation prior to combustion are revealed using dual optical diagnostics

- **Liquid impinges upon wall and forms a terminating film of approximately 30 mm in diameter (10 mm larger than jet diam.)**
  - Fuel film has "texture" indicating non-uniform thickness
  - Overall fuel film thickness is unknown at this stage, but is < 10 μm
- **Significant liquid remains in ambient as a wall jet and does not stick to the wall as a film**
- **Film persists on wall for > 100 ms, during compression heating and while the flame arrives**

Wall conditions

Axial distance	50 mm
Wall diameter	50 mm
Wall Initial T	**102 °C**
prism dimension	40 mm
10° engineering diffuser	

Injector conditions

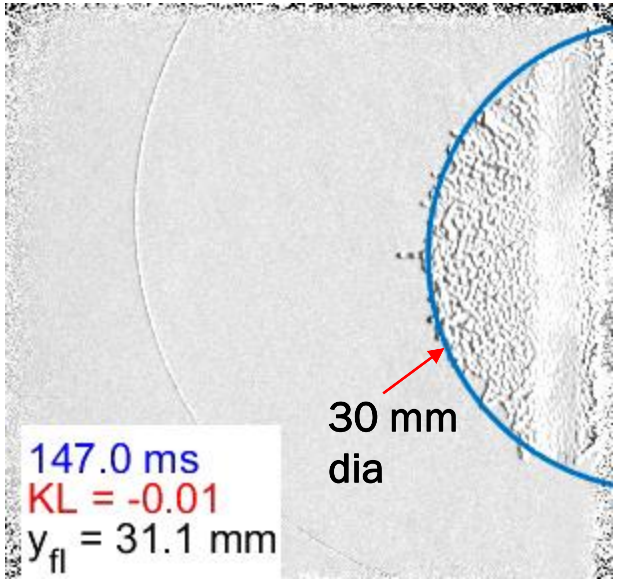
Fuel	**RD-587**
10% ethanol PACE gasoline	
Inj Pressure	350 bar
Inj Duration	2.4 ms
Inj Mass	13 mg
Injector nozzle	single-axial
Nozzle diam.	0.189 mm

Ambient conditions

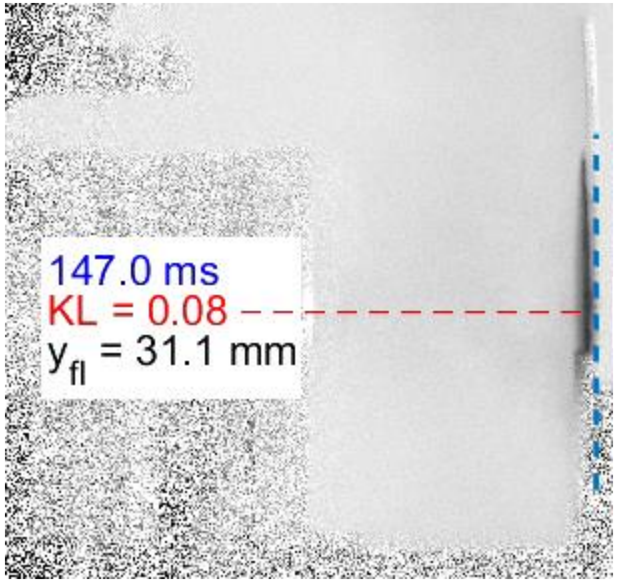
C2H2	3.2 v%
H2	0.5 v%
O2	8.2 v%
N2	13 v%
equiv. ratio	**stoich. dilute**
Initial T	102 °C
Initial P	7.1 bar

- **Temperature of "core" gases away from the wall estimated using adiabatic compression and flame assumptions**

wall-view extinction I/I_0

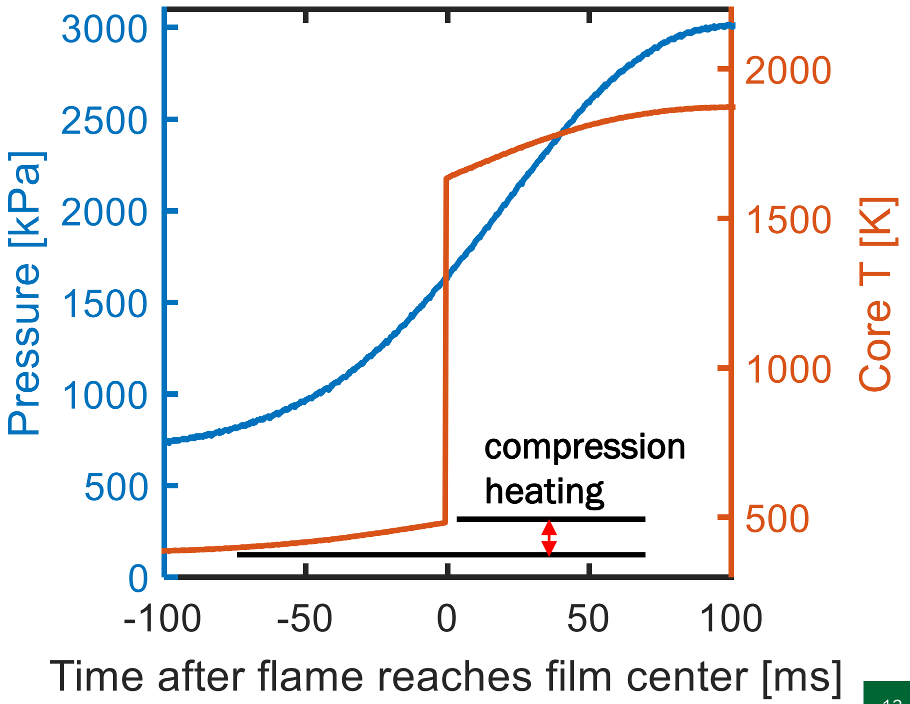


side-view extinction I/I_0



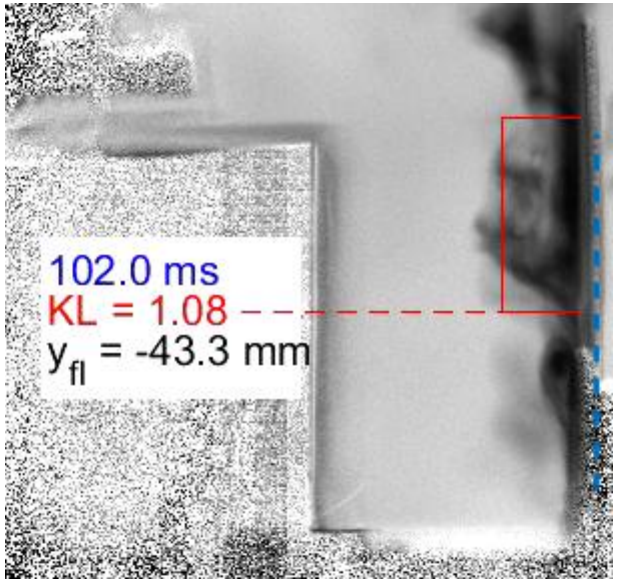
Film visible in side view

30 mm

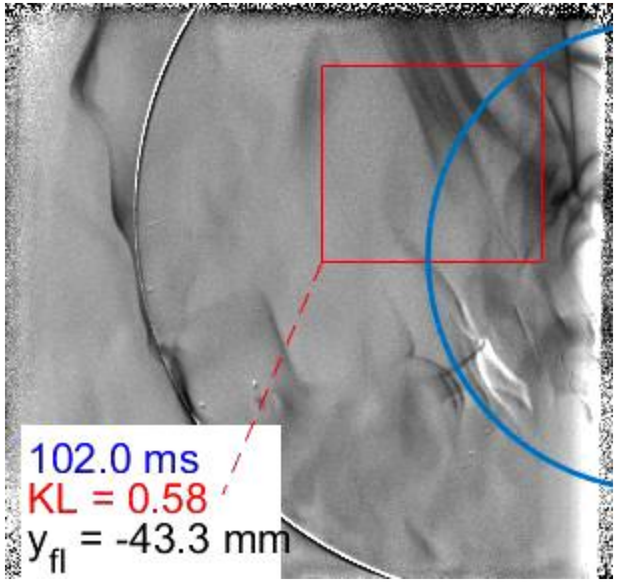


Soot levels quantified as flame moves over film

- **Side-view: mean optical thickness calculated in a 6.7 x 16.4 mm region**
  - Time relative to flame passing CENTER of film; flame position (from OH* and measured P)
  - Beam-steering is visible as flame approaches
  - Film clearly remains along wall until after flame passes
  - No measureable soot until AFTER flame passes
  - Soot forms AWAY from wall (in high T gases)
  - Turbulent boundary layer forms as rising (buoyancy-induced) convective flow forms



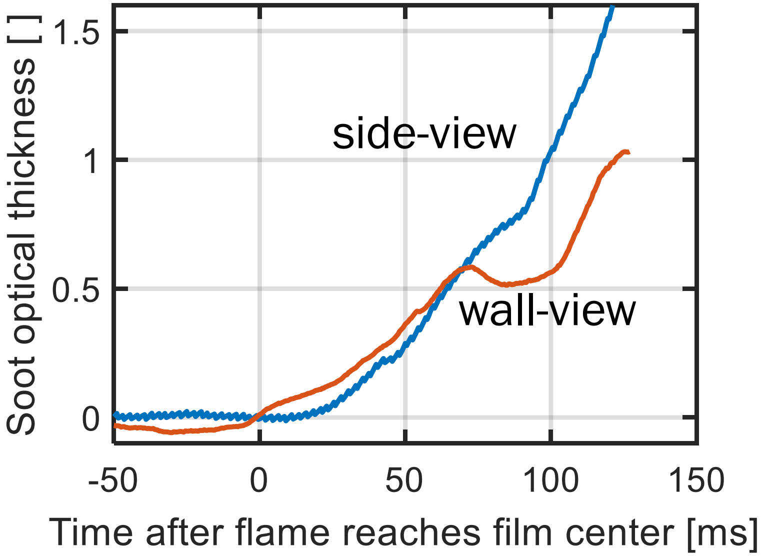
- **Wall-view: mean optical thickness calculated in a 14 x 13 mm region**
  - Beam-steering is more problematic as flame approaches even outside of wall region, but the mean KL is only slightly affected
  - Other results with large-angle diffuser do not have this problem
  - Film texture changes as it vaporizes
  - Soot zones concentrated towards the original film at the center



Opt. Thick. $= \int_{-z}^{-z} f_v(z) \frac{6\pi k_e}{\lambda} dz = KL$

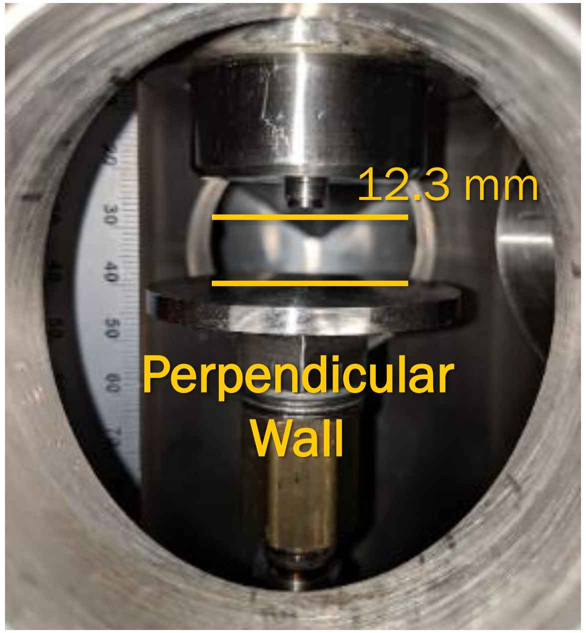
local soot volume fraction

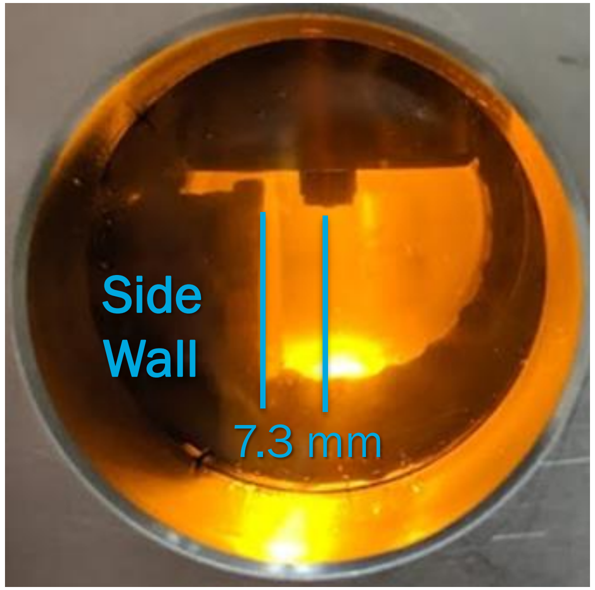
- **Soot increases as T & P increase in core of vessel, even after film appears to be gone**
- **Soot forms SLOWLY in oxygen-deficient ambient, likely contributing to young (and small) particles**
- **Wall temperature and gas temperature in boundary layer expected to be critical for CFD to capture this problem**

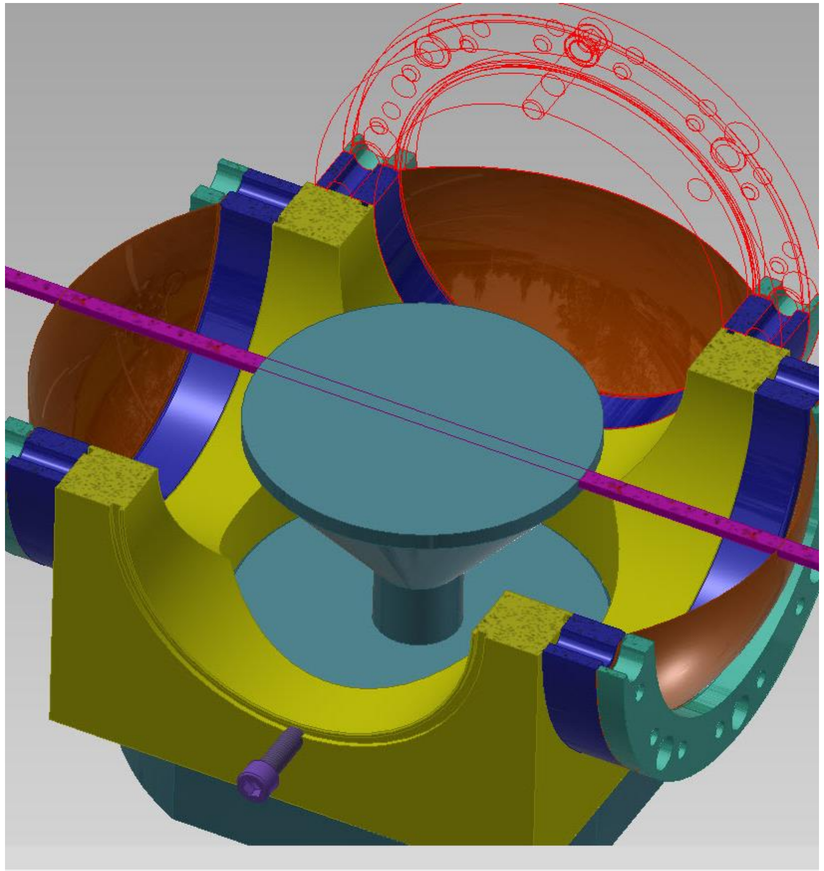


Technical Approach: Exploratory X-ray Experiments with Existing Facilities

- **Several X-ray diagnostics appear promising**
  - Radiography for spray and film density
  - High-speed imaging for morphology and variability
- **Test the diagnostics by modifying existing facilities**
  - Not able to achieve engine-relevant spray/wall distances
  - Allows us to test diagnostics, prioritize future experiments
  - Still useful for model development and validation
- **Design of purpose-built spray/wall chamber is nearly complete**



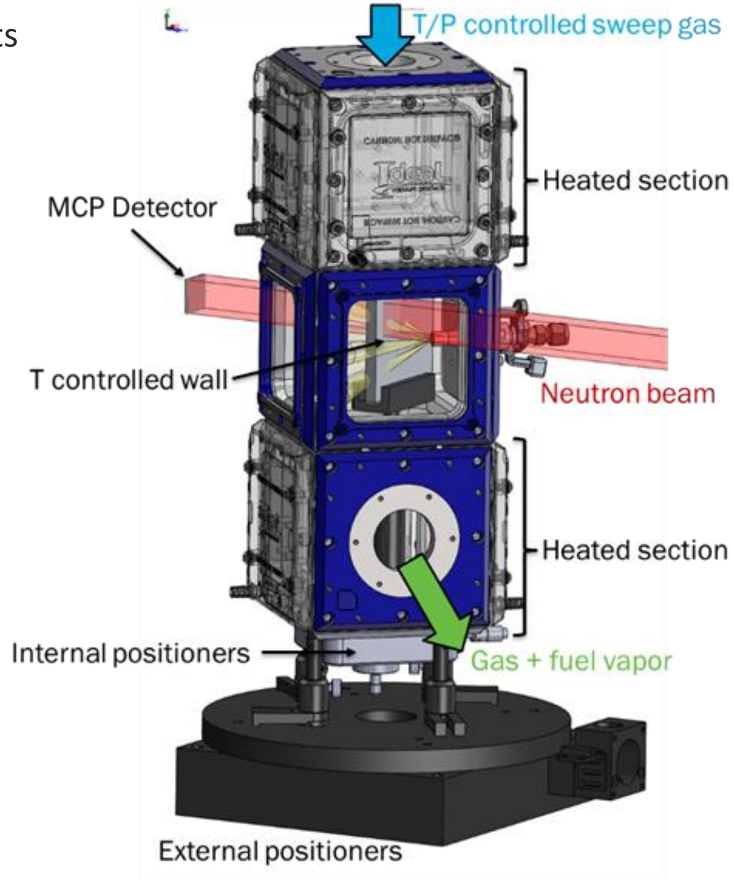




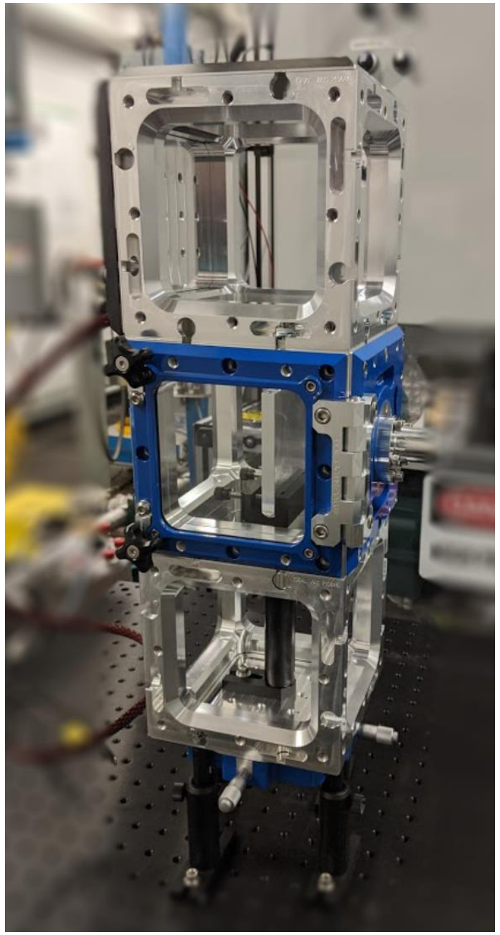
Developing new facility for quantitative neutron imaging of fuel films through metal substrates at PACE conditions

- **Metals have drastically different thermal properties than optically-transparent substrates, which has a significant impact on film deposition and evolution**
- **Facility features**
  - **Chamber:** neutron transparent box, T/P controlled sweep gas
    - Modular design based on commercial vacuum chamber components
    - 6”x6”x6” aluminum cube frame, all faces Al or fused SiO_2
    - Mounted on translation/rotation stage
  - **Wall:** temperature-controlled neutron transparent substrate
    - Aluminum with thermal control via fluorocarbon coolant
    - Option to integrate heat flux probe
    - Mounted on translation/rotation stage inside chamber
  - **Injector:** supports range of GDI-style geometries
    - Fitted through standard NW-25 flange using custom adapter
    - Can be rotated manually, option for future motorized control
- **Diagnostic opportunities**
  - ECN G2 & G3, other “cold” or low-pressure gas conditions (-20 to 150 °C, 0 to 2 bar abs.)
  - Wall temperature 0 to 110 °C
  - View from almost any angle about the vertical axis
  - Many possible injector/wall orientations

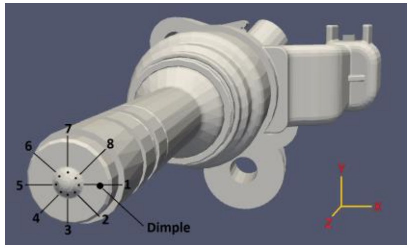
Design concept

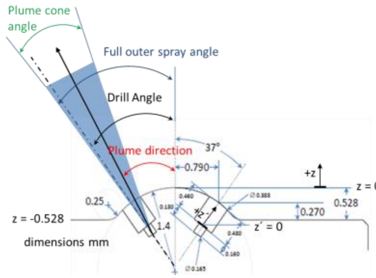


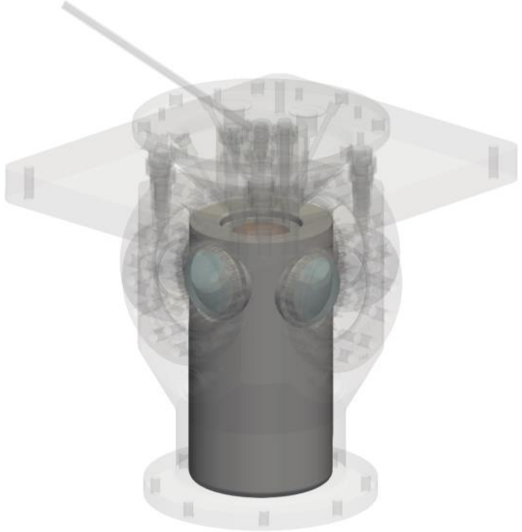
Build progress

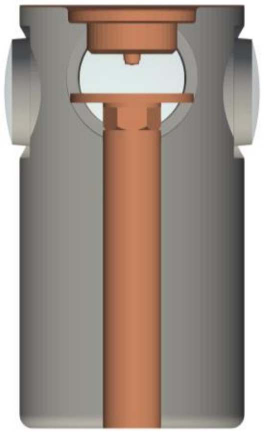


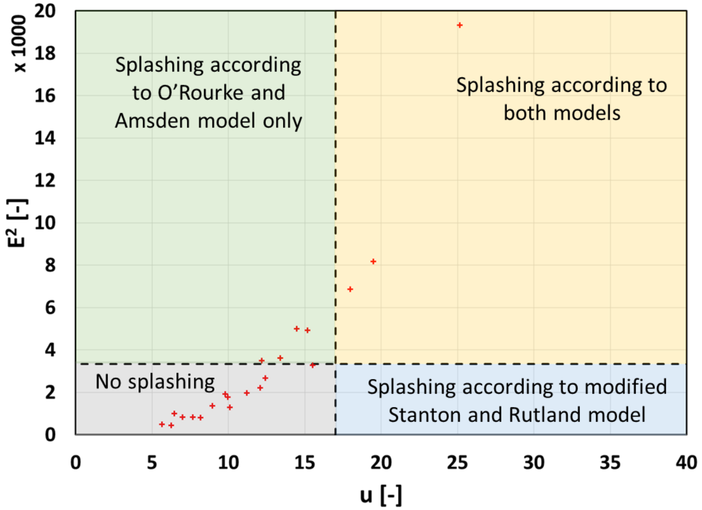
Spray-wall interaction modeling—new method needed for GDI











Impingement frequency of Lagrangian parcels

$$[1, 3]: \quad u = \frac{U_0}{\left(\frac{\sigma}{\rho_l}\right)^{1/4} \nu_l^{1/8} f^{3/8}} > 16-18$$

$$\boxed{[2] \quad f_{imp}(x,y)\Big|_{A_d} = \frac{3}{4}\frac{r_d^2}{r_c^3}\frac{UN_d}{\cos(\theta)}}$$

- Original formulation of Stanton and Rutland[1] SWI model was extensively modified to account for **impingement frequency dynamics, key for solving the chaotic nature of SWI[2]**.
- SWI model implementation in CONVERGE 3.0 is ongoing (full UDF capability in v3.0 was made available in February 2020)
- **Current setup used the O'Rourke and Amsden SWI model[4]**

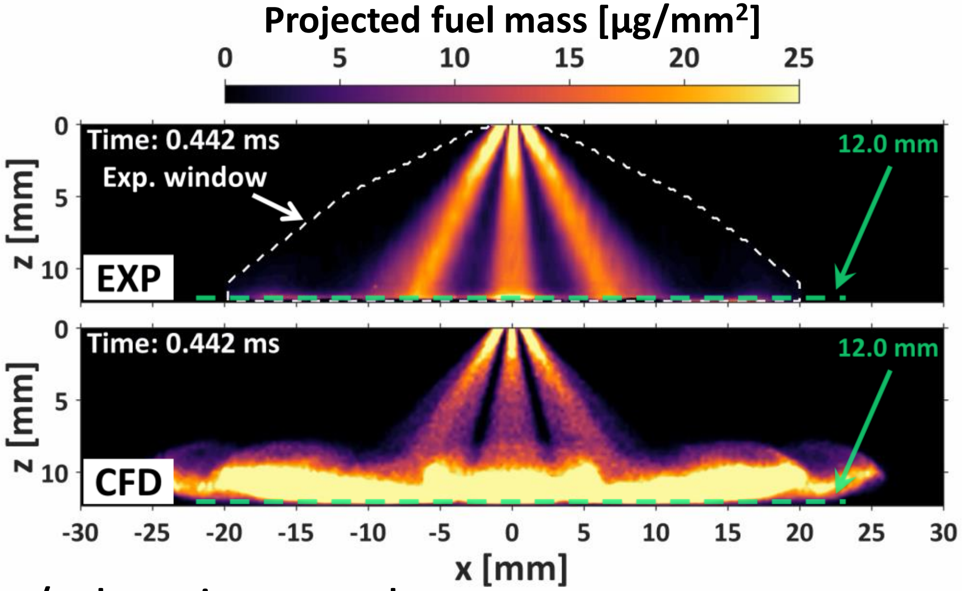
The Spray G injector was used for all the simulations:

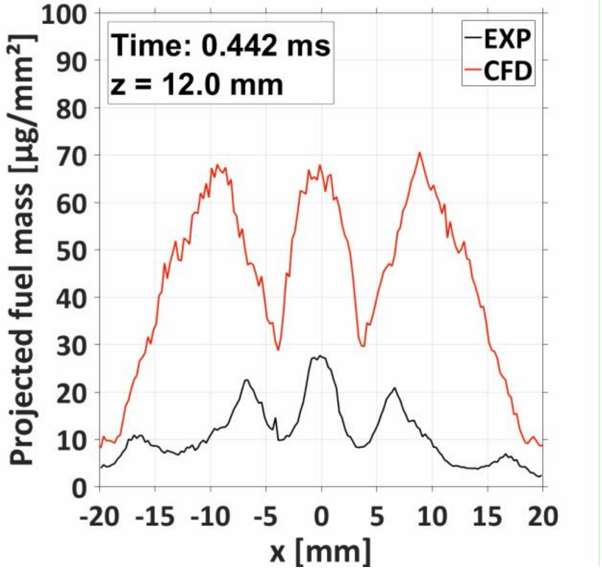
- Work explored use of RNG k-ε model (preferred for ICE simul.)
- A standardized reference system allowed for consistent comparisons between experimental and numerical datasets
- Exact computational domain was modeled after the X-ray chamber (rather than the typical box/cylinder) including details of injector tip and impingement plates
- New, dedicated post-processing tools that can read directly from CONVERGE's output were developed for consistent quantitative comparison against X-ray experiments
- Processing tools/new models can be shared with industry

[1] Stanton and Rutland, SAE 960628, 1996
[2] **Torelli et al, IJER, 2020**
[3] Yarin and Weiss, J. of Fluid Mech., 1995
[4] O'Rourke and Amsden, SAE 961961, 1996

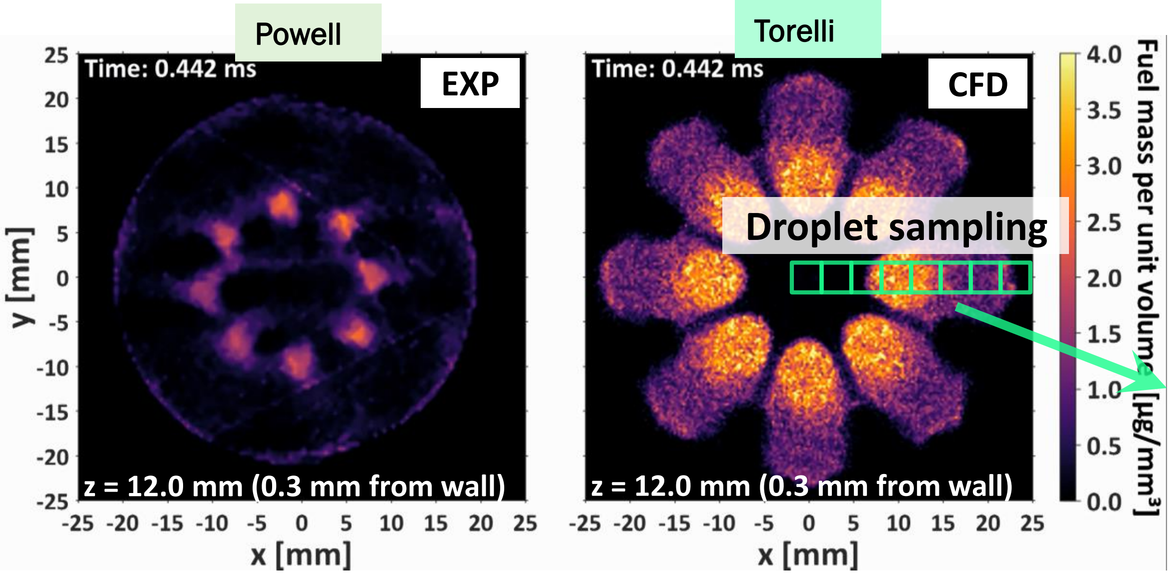
Simulations vs. Argonne's X-ray experiments (front wall)

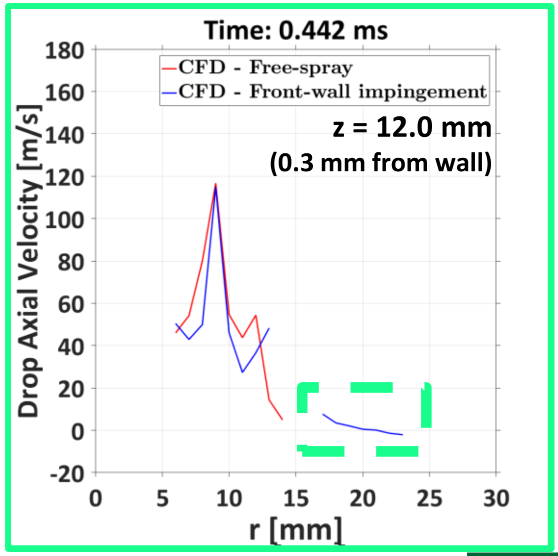
- Setup from free-spray cases applied to G2, G2-cold, G3, and G3-cold cases with spray-wall interaction
- Simulation of G3-cold case (T=298 K, p=100 kPa) with wall located at z = 12.3 mm
- Projected fuel mass showed excellent agreement between z = 0 mm and z = 5 mm
- After the impingement , CFD showed more fuel mass accumulation in the near-wall region than observed in experiments
- Low-velocity, non-impinged droplets appeared in the front-wall case as a result of the interaction of the incoming jet with the near-wall gas highlighting the importance of correct predictions of the near-wall flow field
- Experimental uncertainty exists about the perpendicularity of the plate relative to the injector axis (x = 0 mm)





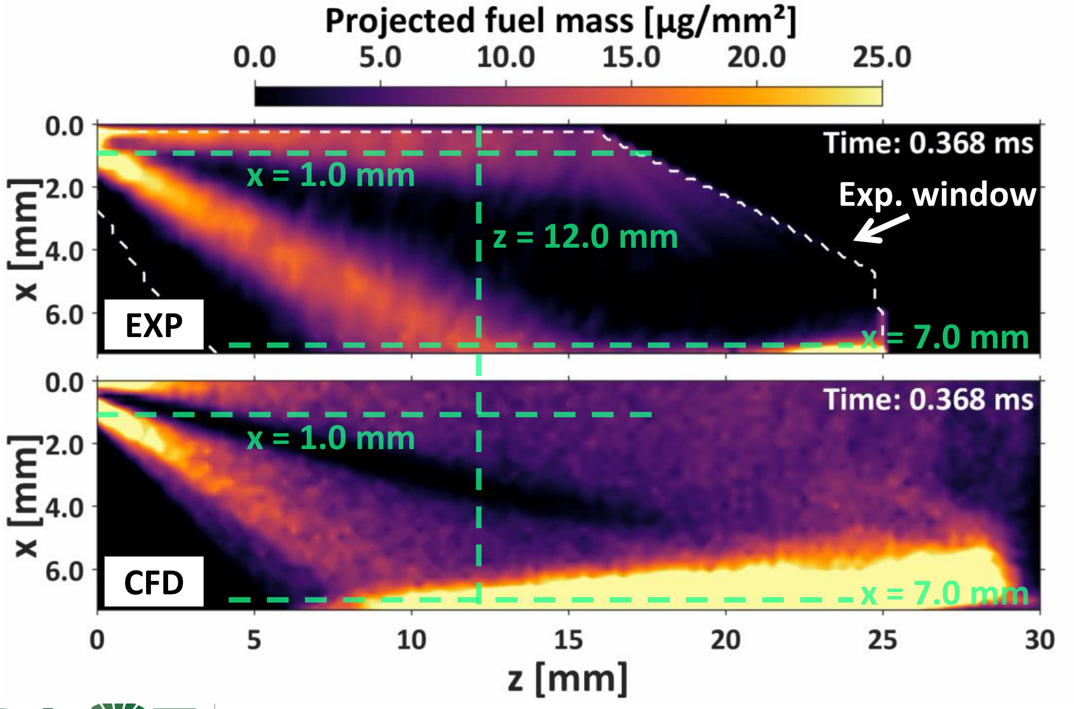
Fuel mass / volume via tomography

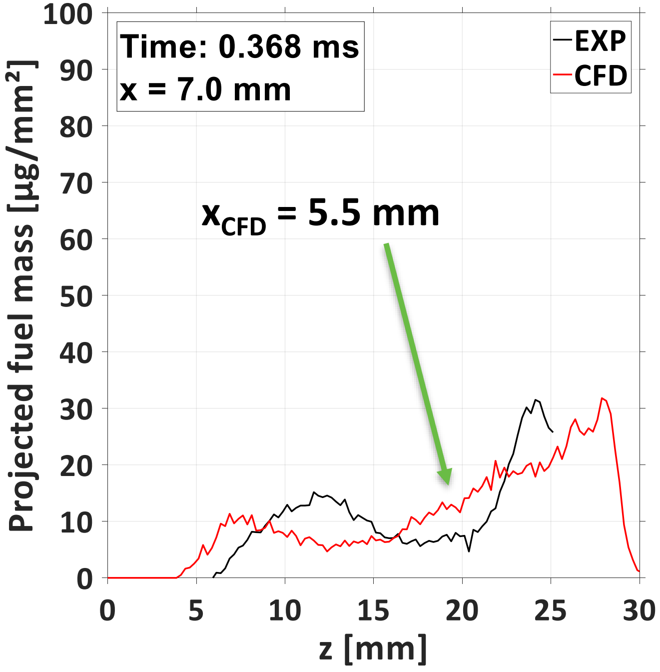


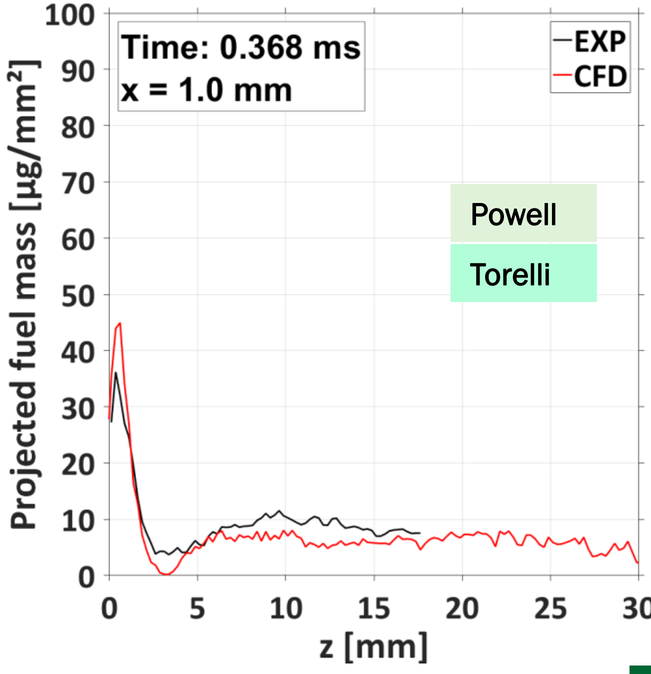


Simulations vs. Argonne's X-ray experiments (side wall)

- Same setup from front-plate cases applied to cases with lateral spray-wall interaction
- Simulation of G3-cold case (T=298 K, p=100 kPa) with side wall located at x = 7.3 mm
- Following the impact of the spray with the wall, simulations showed more fuel mass accumulation in the near-wall region than it was observed in experiments similarly to what occurred in the front-wall cases
- Uncertainties exist with respect to the precise location and orientation of the wall in the experiments, as suggested by the calculated projected fuel mass profile shifted by 1.5 mm. The new experimental setup of Powell et al will address these issues
- Projected fuel mass showed excellent agreement in the free spray region along the whole extent of the spray plume







Powell

Torelli

Approach: Apply multiphase simulations for wall film dynamics via volume of fluids (VOF)

- **Eulerian multi-phase modeling combined with particle method to model the fuel wall-film behavior**
  - Spray G is modeled in the center of 50 mm box by the Lagrangian particle method in (Fig. 1).
  - Particles transform from Lagrangian to Eulerian at the wall (Fig. 2).
    Eulerian frame: momentum, heat transfer and mass transfer, but no vaporization.
    Interface tracked by the Volume of Fluid (VOF) Eulerian method (Fig. 3)
    - Each particle carries the mass, velocity and temperature (energy) phase space information.
    - Interpolate mass, velocity and temperature (energy) to each node:
      - FEM shape functions employed, transition from particles to nodal FEM form.
    - Primary variables calculated by the first principles, conservation of momentum, mass and energy.
  - **No engineering wall-film models, predictive on first principles if interface is resolved accurately**
    - Better accuracy but requires high wall resolution with films on the order of 1 μm. use of FEARCE's h-adaptive or AMR type grid refinement to obtain high resolution when and where needed.
    - Combined with Verman Dynamic LES, which will accurately simulate engines & regimes not accessible otherwise.

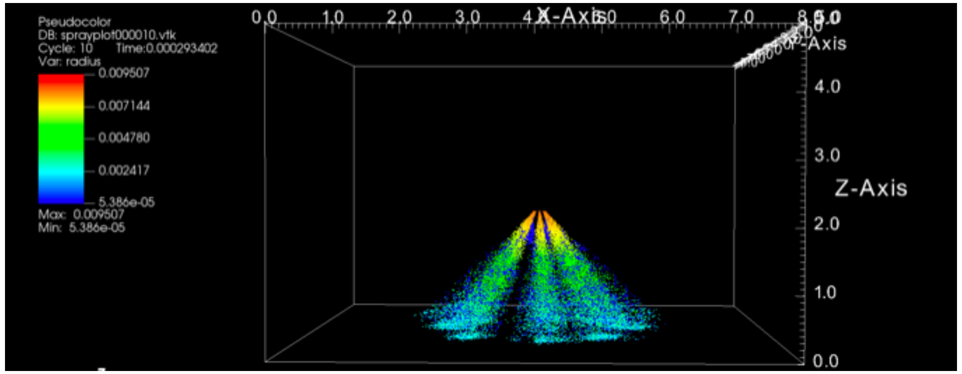


Fig.1 Free-spray modeled by LPT and hit the wall, Particle radius in color

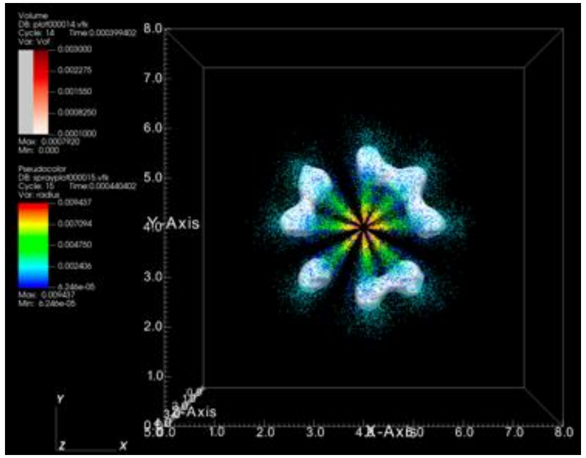


Fig. 2 particle transitions to VOF at the wall. particles (rainbow color) and VOF (gray scale)

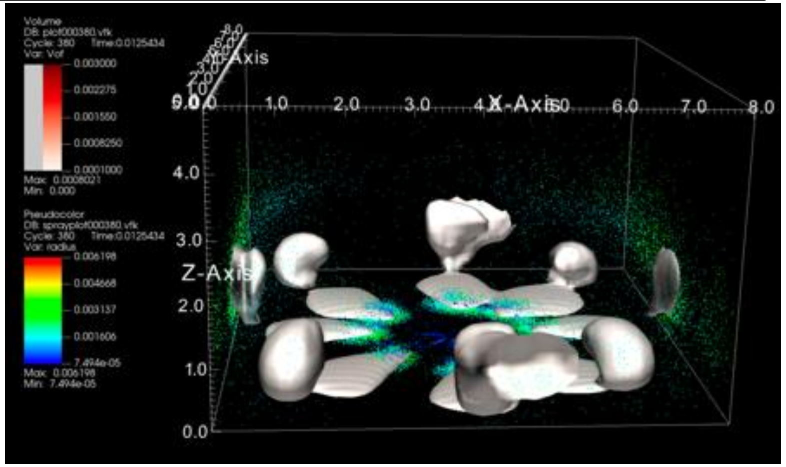
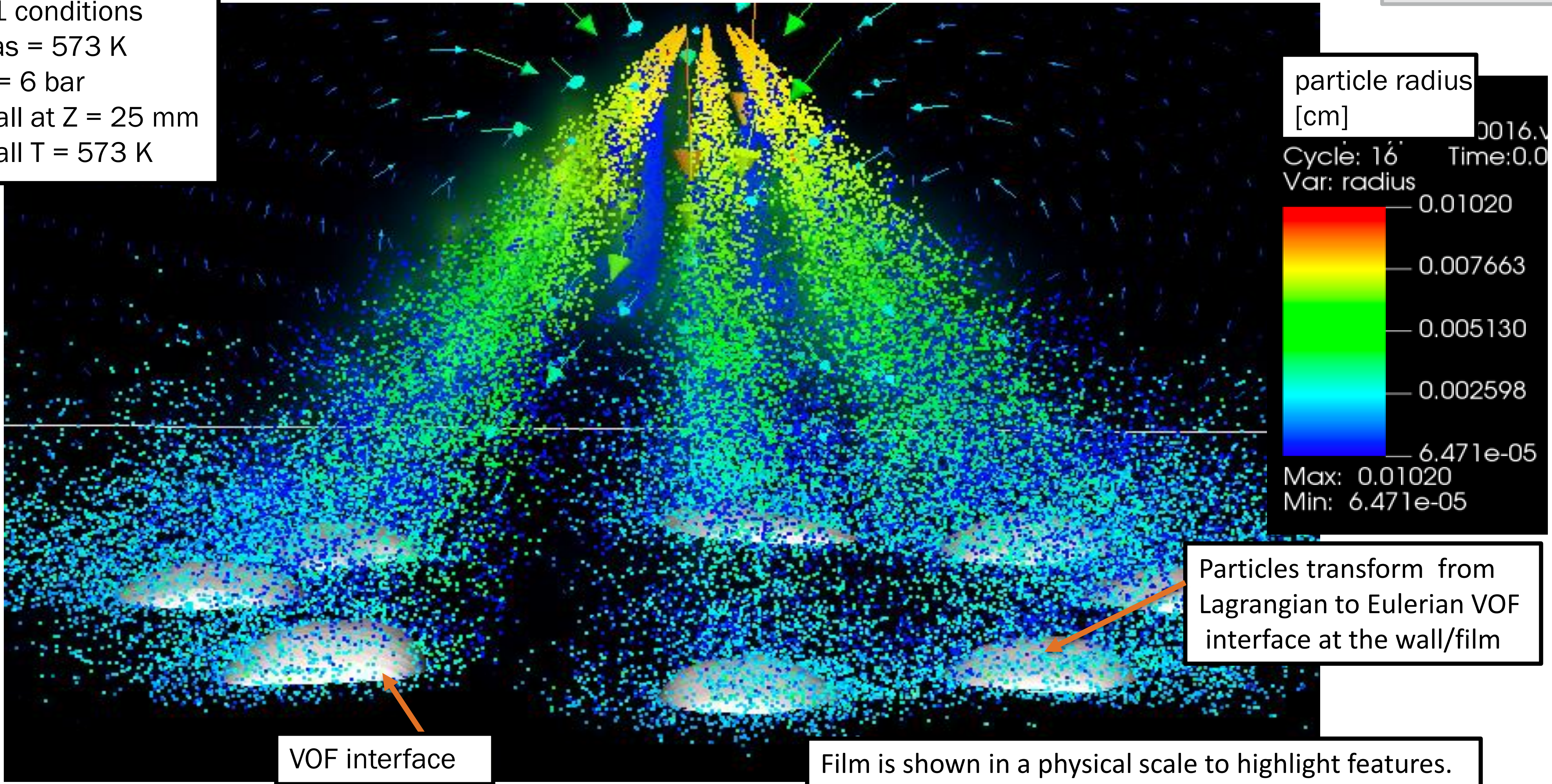


Fig.3 VOF interface tracking of the multi-phase flow at the walls.

Multi-phase Lagrangian-Eulerian methods developed for predictive wall-film modeling: Informing Engineering models in any system (To include vaporization in phase 2)

G1 conditions
Gas = 573 K
P = 6 bar
Wall at Z = 25 mm
Wall T = 573 K



Particles transform from Lagrangian to Eulerian VOF interface at the wall/film

VOF interface

Film is shown in a physical scale to highlight features. Actual film thickness is 1-2 μm

Spray morphology is strongly affected by fuel temperature and engine speed – Challenge for CFD?

- Performed 39 kHz dual-camera spray imaging to:

A) Understand in-cylinder mixture formation.

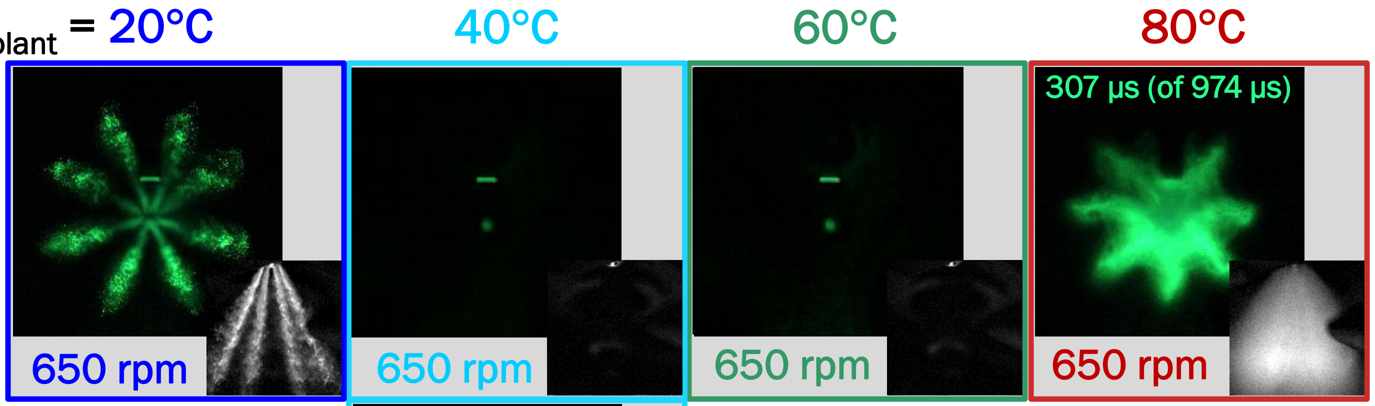
B) Guide spray-vessel experiments.

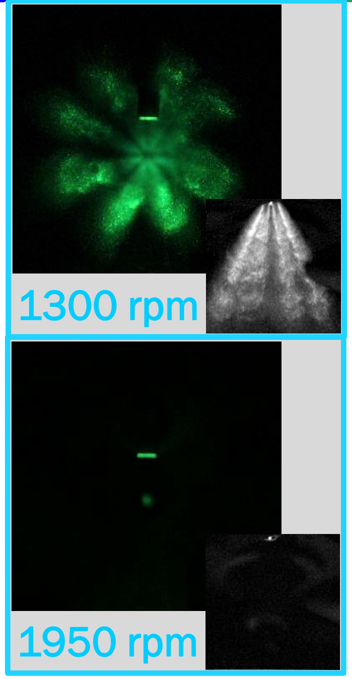
C) Assess gasoline surrogates being developed.

D) Generate database for CFD validation.

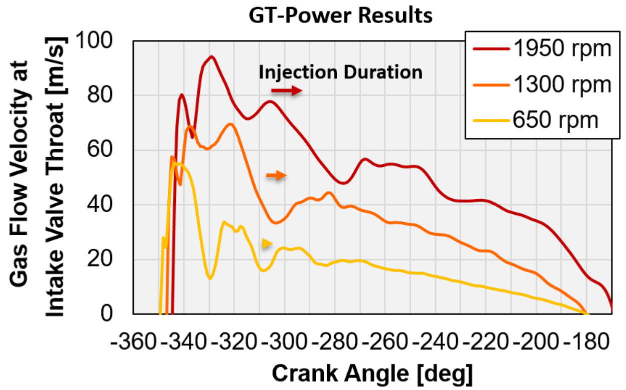
- Large test matrix across ranges of coolant temperature, engine speed, injection pressure, intake pressure, and injection duration.
- For RD5-87, flash boiling becomes active in the 40 – 60°C range ($P_{cyl} \approx 51$ kPa).
  - Improves the atomization process.
  - Allows the use of lower injection pressure?

- **Predictive modeling needs to capture these effects.**





- Increased engine speed can trigger plume interact.
- Strong cross flow causes spray deflection



Collaboration and coordination with other institutions

- **PACE Sprays & Films team meets monthly to coordinate more than 60 different tracked tasks**
  - Decisions about target conditions, including CFD and experimental boundary conditions, are coordinated in advance
  - Data and analysis tools are shared/combined to reach physical conclusions about current models
  - Work is foundational to other PACE objectives in a DOE-funded consortium of 6 National Laboratories working towards a common goal (ACE138)
  - All team members participate in the Engine Combustion Network, an international collaboration with 20+ members and 10+ institutions who have specifically chosen Spray G wall films and combustion as a special topic
  - ECN7 workshop will be held in June 2020 (online web meetings)

Collaboration and coordination with other institutions (detailed)

D.01.05 Pickett	• PACE Sprays Team lead and ECN lead; created online ECN archive for GDI; ECN has chosen wall and film combustion with 20+ volunteer researchers • PACE activities not reviewed here: fuel surrogate selection & blending (Wagnon), cold-start condition sprays (Curran), heat-transfer (Edwards) • Co-Optima participants on GDI fuel effects: experiments with fuel blends shown promising for multi-mode combustion with early- and late-injection
D.01.04 Manin	• ECN and International Energy Agency lead on soot. Working with 6+ active institutions on problems related to soot formation in gasoline and diesel • Actively working with PACE soot modelers Hanson (SNL), Pitz/Kukkadapu (LLNL), using free-jet pyrolysis and oxidative reacting sprays • Re-creating conditions of PACE engine experiments at SNL (Sjöberg) and ORNL (Curran/Edwards) for study of film combustion
E.01.02 Sjöberg	• Co-Optima PI and Team Lead of Advanced Engine Development. • PACE activities not reviewed here: fuel surrogate selection & blending (Wagnon), and cold-start conditions (Curran). • Collaborating with Xu He at Beijing Institute of Technology on fuel sprays, wall wetting and flame-speed measurements. • Collaborating with Charles McEnally at Yale on fuel sooting metrics.
D.01.01 Powell	• Lead for ECN internal flow and near-nozzle behavior for Spray G • Internal collaboration with Argonne X-ray Sciences Division
D.01.02 Wissink	• Coordination with PACE Sprays Team • Injector hardware provided by GM, Delphi, Bosch • Internal collaboration with ORNL Neutron Sciences Directorate to develop new detector hardware and improve quantitative data analysis techniques
D.01.03 Nguyen	• Led in sharing joint processing scripts and facilitating data exchange for PACE modeling with Waters and Torelli for workshops and group meetings • Volunteer for ECN data exchange synthesis with Lucchini (PoliMi) for GDI topic
D.02.01 Torelli	• Implementation of new scripts for comparison with X-rays and development of joint scripts with Nguyen and Waters to enable quick, uniform data analysis • Continuing collaboration with Michigan Tech and UMass-Dartmouth for development of spray-wall interaction models • Active feedback loop with X-ray team at Argonne to ensure insightful and consistent comparisons between experiments and simulations
D.02.04 Waters	• Collaborating with SNL for postprocessing FEARCE spray data by the script provided by Nguyen. • Using experimental spray data provide by ECN for comparison.

Remaining challenges and barriers

- **Free-spray simulations need to be improved to provide quality predictions at the wall**
  - All free-spray simulations to date show higher LVF than in experiments
  - Simulations show high sensitivity to assumptions, not predictions, for plume cone angle
  - Properties and methodology for preferential evaporation with multi-component fuels need to be improved/verified
- **Discovering source of apparently "higher rebound" in spray-wall interaction models**
- **Experiments need to provide improved accuracy in wall & liquid/vapor regions**
  - Optical experiments are highly sensitive to droplet size—sizing measurements are needed at all timings and positions
  - X-ray experiments are difficult at low fuel concentration and need to address vapor fuel and temperature gradients, in addition to liquid fuel
  - Throughput with neutron imaging is inherently limited by flux and time constraints and needs to be coordinated with other tasks to prioritize cases of maximum value
  - Wall and gas temperature control are important
  - Technique to distinguish between wall film and droplets in vicinity needs to be developed

Remaining challenges and barriers (detailed)

D.01.05 D.01.06 Pickett	• Addition of temperature-controlled probe with optical access inside pressurized chamber for film thickness and heat flux measurements • Development of workflow such that all team members process/share/benefit from experiments and simulations, accelerating model development • Experimental data provided thus far exceeds the capacity of simulation team—engine simulations with more complexity and physics are not in range yet
D.01.04 Manin	• Droplet sizing to increase accuracy of extinction diagnostics through all stages of injection • More precise measurements of flame position relative to the film • Quantification of gas temperature and mixture concentration in proximity to wall and film
E.01.02 Sjöberg	• For consistency with spray vessel experiments, need to implement Spray G injector in DISI engine experiments. • To better visualize spray-wall interactions, need to re-design piston with a larger window. • To better understand thermal boundary conditions, need to implement temperature measurements in piston.
D.01.01 Powell	• Existing spray vessel cannot accommodate wall position representative of GDI geometries • Measurements involving long pathways next to surfaces, or in dilute (and evaporative) zones far from the injector where signal-to-noise ratio suffers • Distinguishing between wall film and atomized sections of film/wall jet sprays
D.01.02 Wissink	• Modeling suggests that neutron imaging should be able to resolve fuel films < 10 µm, but this remains to be experimentally verified • Throughput with neutron imaging is inherently limited and needs to be coordinated with other tasks to prioritize cases of maximum value • Hardware permitting accurate temperature and heat flux measurements in concert with neutron imaging
D.01.03 Nguyen	• Predictive spray cone angle emerging from the nozzle for flash-boiling and multi-component fuels • Models show insufficient evaporation for colder fuel compared to experiment • Cross flow condition can influence spray behavior -> challenges toward realistic engine simulation
D.02.01 Torelli	• Uncertainty of experimental projected fuel mass in the near-wall region • No existing model (model constants) can simultaneously capture all measured quantities (SMD, projected mass, gas velocities, etc.) within the experimental uncertainty across all the operating conditions (cold-start, high load, flash boiling, etc.)
D.02.04 Waters	• Need for Eulerian evaporation model, mass and heat flux between phases in multi-phase flow (that is employing VOF as an interface tracking system) while not requiring reconstruction of interfaces. • Higher resolution for accuracy required (use of FEARCE's h-adaptive or AMR type grid refinement). Improved wall-clock or turn-around times => faster linear equation system since most of the time is spent in the linear equation solver -> Kokkos for GPU use of Trilinos

Future work

- **Upgrade of experimental facilities to create conditions for wall-impingement at more relative engine conditions**
  - Chambers have precise wall and temperature control
  - Beam paths move through wall and along wall (optical, x-ray, neutron)
  - Creation of cross-flow environment
- **Experiments to quantify multi-component fuels, including the 7-9 PACE surrogate**
- **Adding models for spray-wall interaction in the latest CFD tools**
- **Simulations with higher resolution and with VOF vaporization to inform engineering models**
- **Engine experiments using Spray G injector with optical diagnostics to quantify velocity, liquid, film thickness, and wall temperature at cold-start and other conditions**

Future work (detailed)

D.01.05 Pickett	• Measurements of free-spray LVF and wall-jet impingement using PACE 7-9 component surrogate fuel • Development of diagnostics for film thickness and speciation within multi-component films • Spray and film experiments using PACE-partner fuel injection equipment (Sjoberg, Dec, Edwards)
D.01.04 Manin	• Soot film experiments and pyrolysis with variation in ambient oxygen concentration (0 – 3%) • Soot measurements from non-wall sources, such as dribble at the end of injection • Provide quantitative pyrolysis and soot film data to PACE modeling partners
E.01.02 Sjöberg	• Install Spray G injector in engine and repeat cold-start emissions and engine performance mapping • Perform wall temperature and heat flux measurements during cold-start • Perform spray and film measurements on surfaces with engine flow and different injection timings
D.01.01 Powell	• Fabricate new vessel suitable for engine-relevant x-ray measurements of spray/wall interactions • 3D measurements of near-wall sprays and wall films, rollup vortex, and film thickness
D.01.02 Wissink	• Perform high-speed neutron imaging of wall wetting and film evolution from multiple viewing angles to obtain quantitative measure of film dynamics on metal substrate at a condition prioritized by PACE and Spray Team partners
D.01.03 Nguyen	• Provide all PACE simulations for review and analysis at ECN7 • Provide new distorted droplet model with enhanced evaporation as a release within CONVERGE 3.0 • Development of preferential evaporation model for gasoline surrogate, including operation specific to flash-boiling conditions
D.02.01 Torelli	• Complete implementation of Argonne's version of Stanton and Rutland's model in CONVERGE 3.0 and improve it based on new x-ray and optical data • Perform multi-cycle simulations of SIDI optical engine, evaluating quantities for isolated wall jet experiments. Document "best practices" for simulations
D.02.04 Waters	• Model the internal flow of the injector with VOF • model the boundary layer heat transfer with LES • compare the wall film results by VOF against the experimental data and particle methods

Any proposed work is subject to change based upon funding levels

Summary

- **Combined and complementary optical, x-ray, and neutron experiments offer the potential to advance understanding and CFD of free-spray and wall-impingement physics**
- **Experiments show that wall temperature and realistic gasoline fuel (multi-component) are the most important factors for emissions during cold start**
- **The outcome of wall films and a stoichiometric flame is slow, delayed soot formation after fuel vapor escapes from wall into a hot core away from wall**
- **Comparison between proof-of-concept wall impingement experiments and current CFD capability already reveals paths for needed future CFD development directions**
  - Higher liquid vaporization is needed
  - Predicted wall rebound is greater than experiment

Summary (detailed)

D.01.05 Pickett	• Free spray experiments with multiple injections provide downstream 3D liquid volume fraction to understand likelihood of wall wetting • Measurements show the strong effect of multi-component fuels representative of gasoline, affecting plume interactions and final vaporization
D.01.04 Manin	• Unique and quantitative experiments demonstrate the phenomenological processes of soot formation from wall films and stoichiometric combustion • Soot forms very late after flame passes over film, as fuel vapor is transported into hot regions and undergoes pyrolysis • Datsets are targets for PACE combustion team
E.01.02 Sjöberg	• Scoping studies at cold-start conditions identify the most important parameters affecting PM formation: fuel type, wall temperature, injection schedules. • In-cylinder visualization shows strong effect of intake cross flows on spray collapse, demonstrating that engine flows must be incorporated to understand wall wetting
D.01.01 Powell	• Proof of concept experiments have shown that x-ray diagnostics can generate unique, quantitative measurements of spray/wall interactions
D.01.02 Wissink	• Recent high-speed neutron imaging experiments have directly visualized GDI spray/wall impingement and fuel film evolution looking through aluminum • Facility specifically for quantitative neutron imaging of fuel films through metal substrates has been designed and construction is in progress • Plans going forward are to perform quantitative measurements of film evolution on metal substrates at PACE conditions
D.01.03 Nguyen	• A methodology to understand the "threat" of liquid impingement has been developed for free spray simulations, specifically showing multi-component fuel composition and fuel temperature effects on persistence of liquid mass at given wall positions
D.02.01 Torelli	• New spray setup coupled with RNG k-eps turbulence model led to good matching of simulations against quantitative X-ray data of fuel mass using readily available spray-wall interaction models • CFD is pointing at possible ways to improve experimental diagnostics
D.02.04 Waters	The mass, momentum and heat transfer in the Eulerian phase is modeled from 1st principles, removing engineering models for fuel forming films on walls. The multiphase flow, compressible gas and incompressible liquid film are tracked with the VOF method. Eulerian multiphase modeling reduces computational time by not requiring tracking of particles on the wall.

Technical Back-Up Slides

Complete PACE Budget

Combustion and Kinetics Team

		Lab	PI	FY19	FY20
A.01.01	Improve kinetic models for gasoline surrogates for combustion control, cyclic variability, and emission reduction	LLNL	Pitz	$325k	
A.01.02	Improved Kinetics for Ignition Applications	LLNL	Pitz		$150k
A.01.03	Kinetic models for improved prediction of PAH/soot for emission reduction	LLNL	Pitz		$200k
A.01.04	Kinetic models with improved EGR behavior for impact on cyclic variability and combustion control	LLNL	Pitz		$200k
A.01.05	New/improved kinetic models for gasoline components for emission reduction, combustion control and cyclic variability	LLNL	Pitz		$150k
A.02.01	Accelerated multi-species transport in engine simulations	LLNL	Whitesides		$275k
A.02.02	Improved chemistry solver performance with machine learning	LLNL	Whitesides	$175k	
A.02.04	Scalable performance and CFD integration of ZERO-RK	LLNL	Whitesides		$275k
A.02.05	Towards exa-scale combustion simulations with real fuel kinetics	LLNL	Whitesides	$150k	
A.03.01	Autoignition fundamentals at dilute gasoline conditions	ANL	Goldsborough	$450k	$450k

Heat Transfer Team

		Lab	PI	FY19	FY20
B.01.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	$1057k	$100k
B.01.03	Predictive heat and mass transfer modeling in engine systems	LANL	Carrington	$200k	$100k
B.02.01	Accelerating predictive simulation of internal combustion engines	ORNL	Edwards	$200k	$400k

Ignition and Kernel Formation Team

		Lab	PI	FY19	FY20
C.01.01	Advanced Ignition to Enable Alternative Combustion Modes	SNL	Ekoto	$370k	$420k
C.01.02	Fundamental experiments of ignition	SNL	Ekoto	$100k	$420k
C.02.01	SNL DNS/Modeling – Dilute spark ignition	SNL	Chen	$50k	$100k
C.02.02	ML-based Ignition Model Process Development	NREL	Grout		$275k
C.02.03	Turbulence Chemistry Interaction and Ignition Modeling	SNL	Nguyen	$80k	$100k
C.02.04	Development/validation of simulation tools for advanced ignition systems	ANL	Scarcelli	$400k	$400k
C.02.05	Development of spark plasma ignition kernel and flame models	LANL	Mahamud	$0k	$100k

Sprays and Wall Films

		Lab	PI	FY19	FY20
D.01.01	Studies of fuel injection for LD Engines	ANL	Powell	$200k	$200k
D.01.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	$50k	$200k
D.01.03	Droplet Dynamics	SNL	Nguyen	$200k	$100k
D.01.04	GDI Particulates	SNL	Manin	$570k	$500k
D.01.05	GDI spray effects on cyclic variability and cold start	SNL	Pickett	$380k	$380k
D.01.06	GDI sprays leadership & data sharing	SNL	Pickett	$140k	$140k
D.02.01	Towards predictive simulations of GDI Sprays	ANL	Torelli	$300k	$300k
D.02.02	Simulate free sprays in chamber and engines	LANL	Waters	$200k	$200k
D.02.03	SNL Modeling – Simulations of Wall Wetting and Soot Formation	SNL	Nguyen	$100k	$100k
D.02.04	Multi-phase methods and models for predictive simulations of spray behavior: break-up, wall-film, mixture formation, heat and mass transfer	LANL	Waters	$400k	$400k

Lean and Dilute Combustion

		Lab	PI	FY19	FY20
		ANL	Rockstroh	$600k	$600k
F.01.02	Effectiveness of EGR to mitigate knock throughout PT domain	ORNL	Szybist	$125k	$220k
F.01.03	Fuel spray wall wetting and oil dilution impact on LSPI	ORNL	Splitter	$100k	$220k
F.02.01	Developing a framework for performing high-fidelity engine simulations using Nek5000 code	ANL	Ameen	$700k	$700k
F.02.02	Multimode combustion phasing control	SNL	Dec	$280k	$280k

Emissions Reduction

		Lab	PI	FY19	FY20
E.01.01	SI Cold Start	ORNL	Curran	$125k	$350k
E.01.02	Spray flow interaction, mixture formation, and combustion in an optical DISI Engine	SNL	Sjöberg	$135k	$270k
E.02.01	DNS/Modeling of soot emissions from wall films during cold-start and for fuel efficient lean/dilute stratified SACI-like combustion	SNL	Chen	$50k	$100k

Crosscutting

		Lab	PI	FY19	FY20
G.02.01	Machine learning and deterministic patterns	ORNL	Kaul	$150k	$200k

Budget input from team members

- **Timeline**
  - All projects started mid-2019 and are expected to continue to 2023

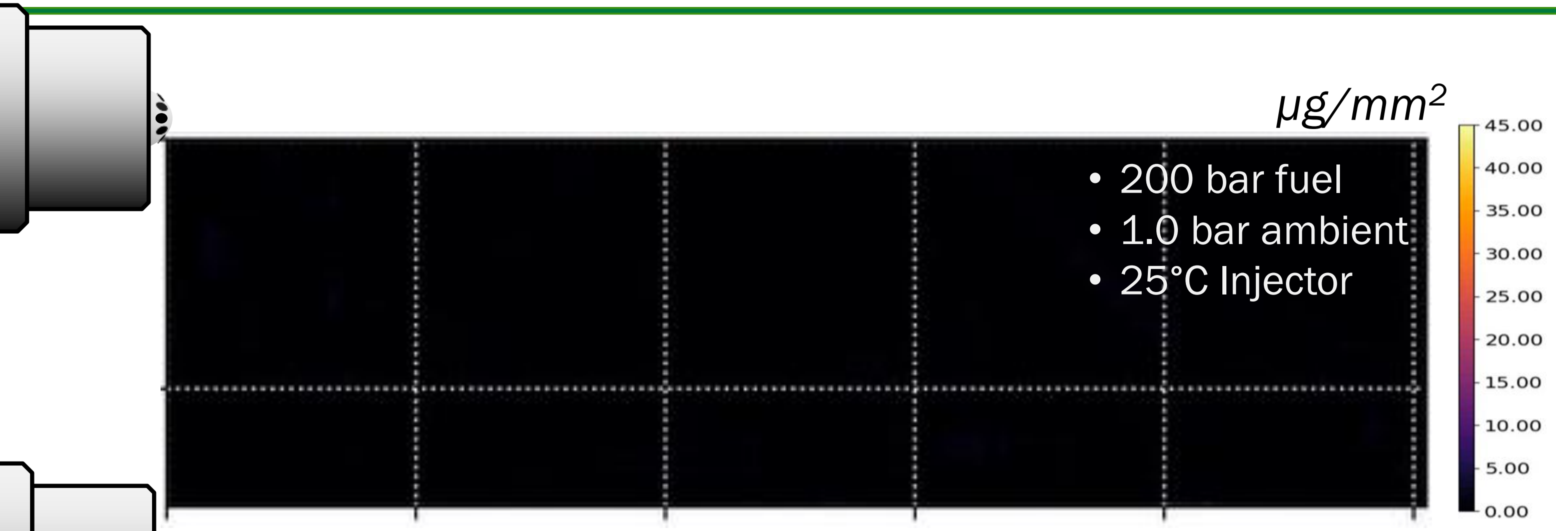
experimental

modeling

Task	Description	FY19	FY20
D.01.05 Pickett	SNL, Free spray and wall film optical experiments Pickett, Skeen, Manin, Hwang, Cenker, Maes	$380	$380
D.01.04 Manin	SNL, Soot and film combustion Manin, Skeen, Pickett, Cenker, Maes, Sim	$570	$570
E.01.02 Sjöberg	SNL, DISI metal and optical engine experiments Sjöberg, Kim, Vuilleumier, Reuss	$135	$270
D.01.01 Powell	ANL, Free spray and wall film x-ray experiments Powell, Sforzo, Tekawade	$98	$490
D.01.02 Wissink	ORNL, Spray impingement and wall film neutron imaging experiments; Wissink	$47	$200
D.01.03 Nguyen	SNL, Evaporative free spray and soot film combustion modeling; Nguyen, Tagliente, Pickett, Chen	$200	$100
D.02.01 Torelli	ANL, GDI spray-wall interaction modeling Torelli, Som	$300	$300
D.02.04 Waters	LANL, Multi-phase methods and models for predictive simulations of spray behavior: break-up, mixture formation, wall impingement, engine heat and mass transfer processes and spark plasma and flame kernel models; Waters, Mahamud, Carrington, Jariwala	$600	$600
D.01.06 Pickett	SNL, Spray team coordination, data sharing, ECN lead Pickett, Maes, Hwang, Prisbrey, Nguyen, Tagliante	$140	$140

Budgets represent total work for PACE project, rather than effort discussed in this presentation

Technical Accomplishment: Density and High-Speed X-ray Imaging



- **Measurements performed for flash-boiling and cold conditions**
- **X-ray Radiography**
  - Measures density in free spray, even in dense near-wall region
  - Can capture vortex formation, extensible to 3D
- **High-speed X-ray Imaging**
  - Camera requires small field of view (0.5 x 1 mm), forces “mosaic” image
  - Time resolution (10 μs) insufficient to freeze spray during steady-state
  - Shows plume impact, drop recoil, film development and flow across wall

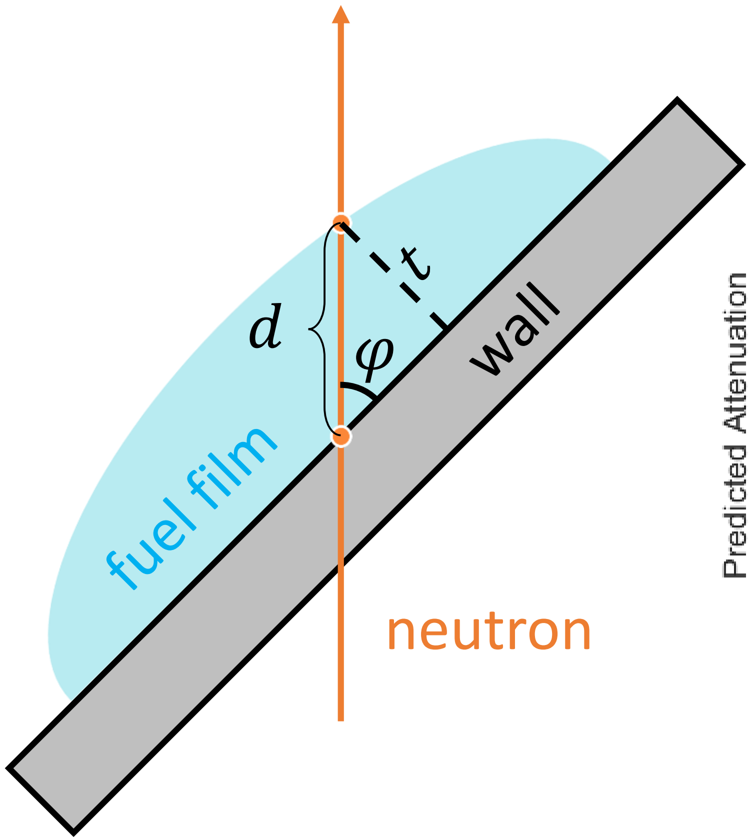
Lessons Learned:

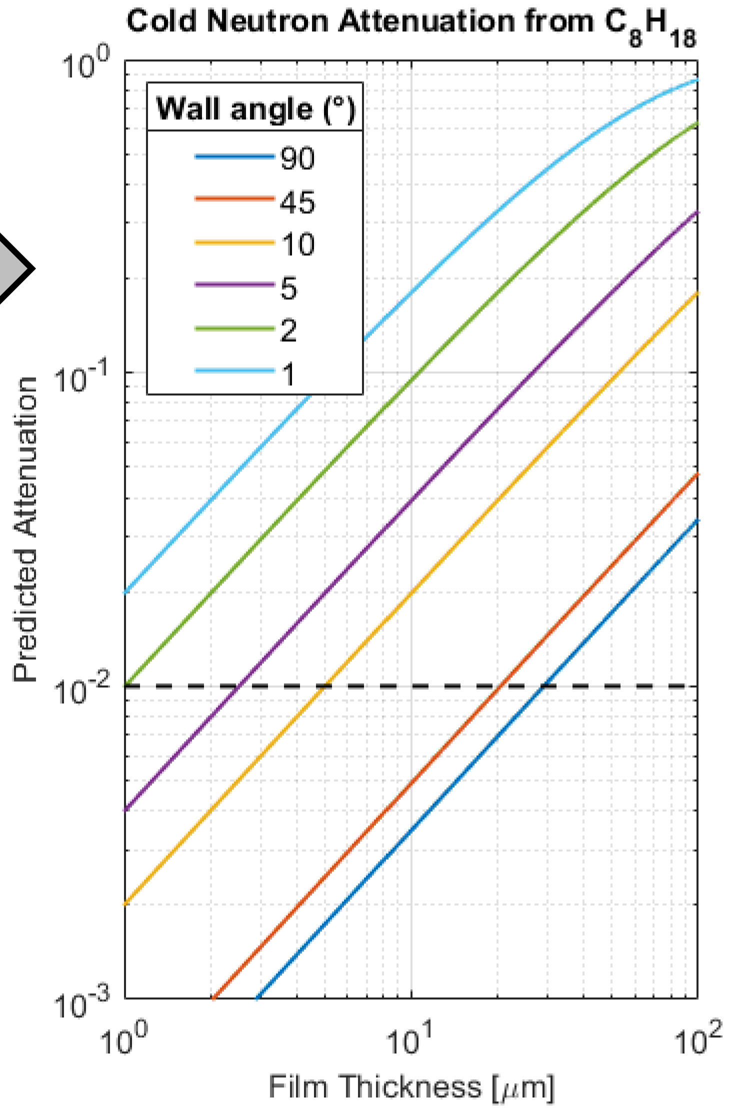
- **Uncertainty of wall position is too large -** New vessel will allow fine control of wall tilt
- **Radiography will be emphasized –** We will explore faster time resolution for imaging

D.01.02: Neutron imaging of advanced combustion technologies (Wissink)

Neutron imaging for film thickness measurement

- Attenuation from ^1H in fuel, no tracer, not sensitive to chemical composition (for similar H/C) or temperature
- Can see through metal walls (80% transmission through 20 mm Al)
- Potential to resolve films down to ~30 µm in normal orientation, ~1 µm if tilted
- Must integrate over millions of injections due to limited neutron flux, 15-30 hr @ 50 Hz for each condition
- Develop technique in spray chamber, long-term intent to measure in engine

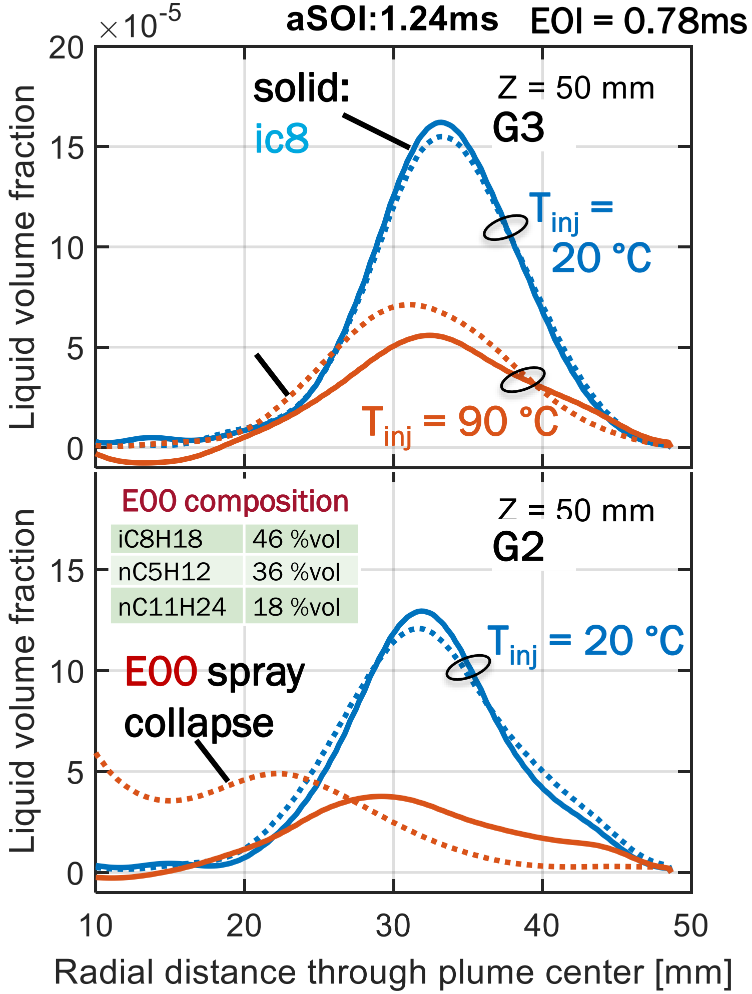




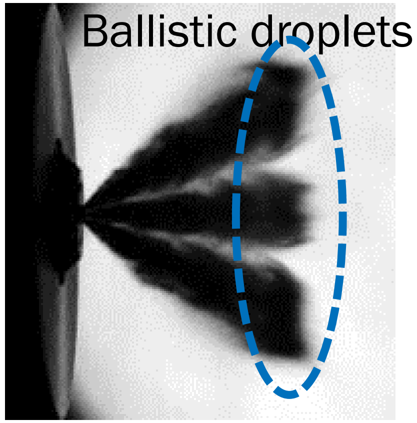
D.01.05
Pickett, SNL

Fuel temperature strongly affects liquid concentration at potential wall positions

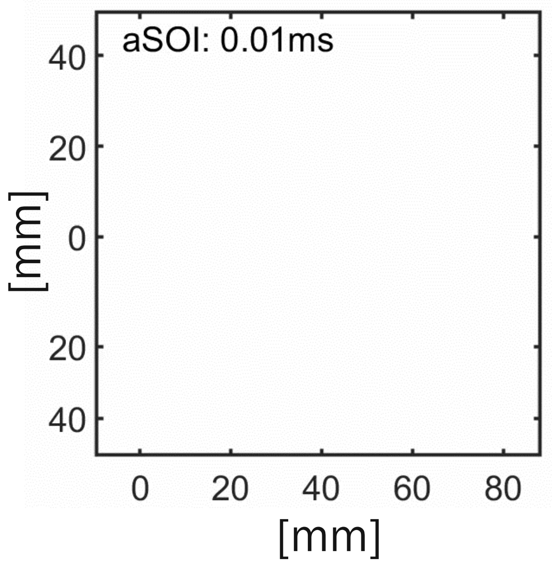
- **At a likely wall position (50 mm), an increase in fuel temperature from 20 °C to 90 °C reduces the liquid volume fraction by ≈ a factor of 3**
  - Examine average of cut planes through center of plumes at wall position in right Figure
- **With cold fuel, single-component iso-octane may have higher liquid volume fraction compared to multi-component (E00) despite much lower boiling point**
  - Volatile fuel components (n-pentane) compensate and vaporize
  - Overall vapor pressure is higher for E00
  - Iso-octane penetrates just as far as E00 (see projected liquid volume movie)
- **Trajectory of plume varies little between fuels at cold conditions, but is very different at flash-boiling G2 conditions with hot fuel**
  - Spray collapse to injector centerline observed for E00 at G2 conditions

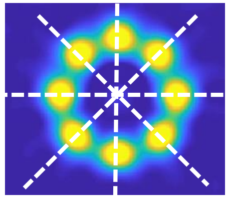


Cold G2
285 us
aSOI



Cold G3
PLV 2e-3

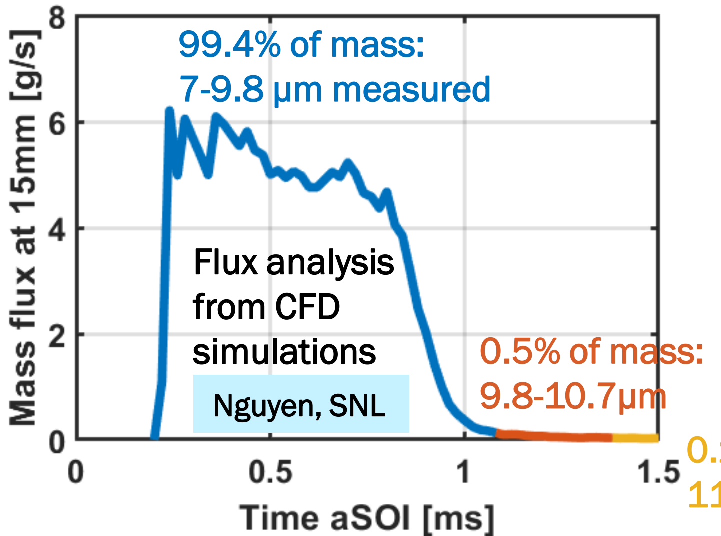


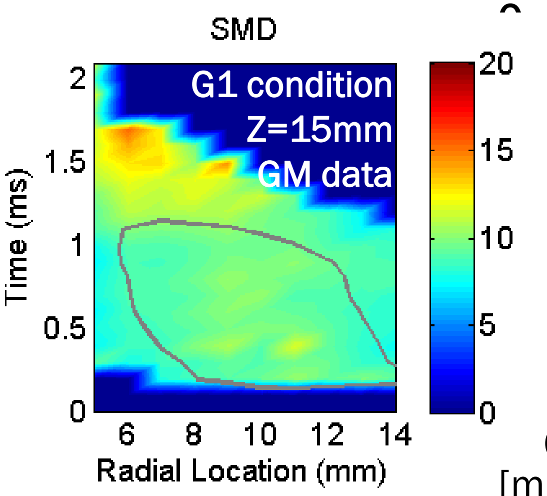


mean of all 8 plumes at an axial cut plane:
Z = 50 mm

Liquid vaporization time-history added as supporting information to preferential vaporization measurements of E00 fuel

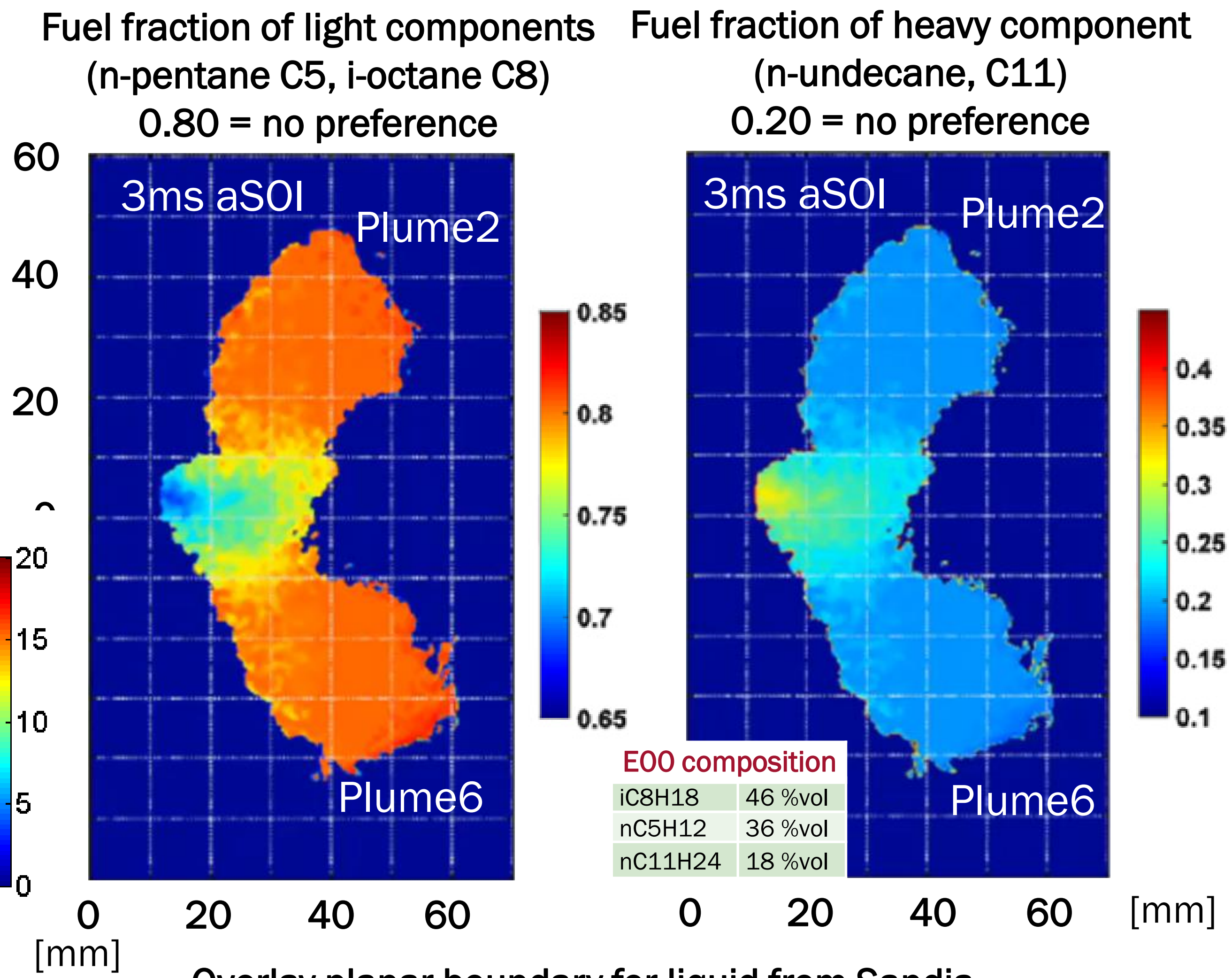
- **Background: How important is preferential vaporization for GDI sprays? What fuel is present at spark plug?**
- **IFPEN performed dual-tracer LIF experiments for G1-E00**
  - One tracer marks light fuel: n-pentane and iso-octane
  - One tracer marks heavy fuel: n-undecane
  - Largest preferential vaporization measured for fuel near injector
- **Planar LVF measurements show final vaporization in the near-injector region**
  - **indicates preferential vaporization for last-injected fuel**
- **Measurements show larger droplet size for last-injected fuel**
- **Our analysis shows MOST fuel charge originates from small droplets**





Planar LIF measurements by IPFEN

G1-E00 conditions Cordier et al., IJER2020, Vol. 21(1) 185–198



E00 composition

iC8H18	46 %vol
nC5H12	36 %vol
nC11H24	18 %vol

Overlay planar boundary for liquid from Sandia measurements with a LVF threshold = 0.5e-6